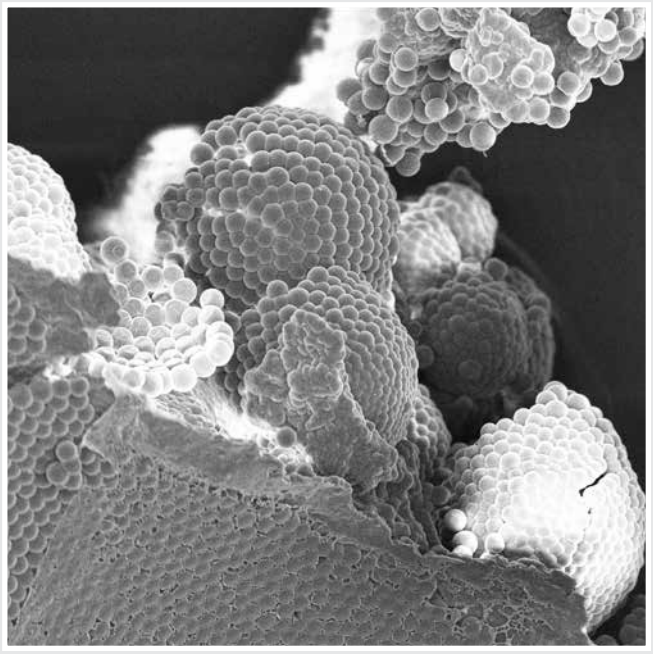
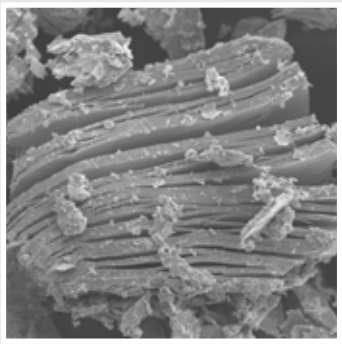
CENTER FOR NANOSCIENCE
ANNUAL REPORT 2017





CeNS
Center for NanoScience | LMU

CONTENTS

CENTER FOR NANOSCIENCE
ANNUAL REPORT 2017

WELCOME

Only one more year to go! In 2018 the Center for NanoScience - CeNS, a grassroots movement dedicated to exploring the nano-world - will celebrate its 20th birthday. Since its foundation in 1998 CeNS has provided a dynamic platform bringing together researchers not only from physics and chemistry, but also from the biomedical sciences, with the aim of facilitating and enhancing the inherent interdisciplinary and collaborative nature of research at the nanoscale.

From the start, the hallmark of CeNS has been a small-scale budget and administrative staff to nurture a special kind of human capital, namely a platform connecting like-minded people with diverse scientific backgrounds and at different stages of their scientific careers. The challenge is to facilitate the transfer of technology between the different disciplines, linking experimentalists and theoreticians, academic research and industry, thus providing a scientific hotbed for the development of new ideas and lines of research in the nano-world. A key aspect of this endeavor is that there is no specific scientific agenda. This ensures that this platform remains flexible, adaptable and always open to new scientific ideas and developments.

Does this approach work? And more specifically, what happened during the last year? The large number of highly competitive grants and awards, international cooperations, and spin-offs linked to CeNS speak for themselves. The latest ERC starting and advanced grants awarded to Alexander Högele, Alexander Urban and Thomas Carell, or the renewal of the SFB863 are just a few examples. The CeNS community keeps growing and we are very happy to welcome our new members Christof Mast in the Physics Department and Ulrich Lächelt in Pharmaceutical Biotechnology, and to welcome back Philip Tinnefeld who joined the Department of Chemistry, as well as Thorben Cordes who generates new links to the Biology Department. New ideas need seed funding and CeNS has provided financial support for seven new cooperative projects between CeNS groups and also supported shared infrastructure heavily used by the CeNS community.

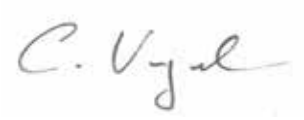
A particular highlight of the CeNS 2017 calendar was the four-day International Conference on Enhanced Spectroscopy organized by Achim Hartschuh in Munich, with CeNS and NIM acting as hosts. The conference attracted 100 participants and speakers from all over the world, endorsing the international standing of Munich Nanoscience. A further highlight was the Annual Conference in Venice, this time co-organized by CeNS and the SFB1032. The theme of the meeting was Design and Control of Nanosystems and, once again, all participants were housed on the island of San Servolo, encouraging exchange between students, CeNS members and international speakers.

A central focus of CeNS is to provide as many opportunities as possible for international exchange and initiative, in particular at the graduate student and postdoc level. With the support of Jan Lipfert, who arranged for the University of Illinois at Urbana-Champaign to act as the partner institution, CeNS organized the Junior Nanotech Network (JNN) with 11 participants from Germany and the US who took part in a two-week mixed scientific

program of lectures and hands-on lab experience in Munich. Responsible for organizing Science in a Nutshell, the welcome event for new CeNS PhD students and the ever-popular Seminar Series Science Rocks!, the students also initiated workshops on Adobe Illustrator and Visual Communication. Contacts between university and industry were fostered through several events, including the CeNS company visits to Roche and to the spin-off Nanion, as well as the workshop "Patents - How To Protect Your Ideas" and the CeNS Meets Industry event. The latter was followed by the annual CeNS Summer Party and the B2Run with more than 20 resilient contenders thriving under the CeNS banner against a fierce competition in a 6 km run through the Olympic Park.

The format of the CeNS awards for travel and for publications provides an attractive opportunity to highlight achievements and to promote the visibility of this enterprise. As ever it was one of the most difficult but also pleasant duties of the CeNS board because of the high quality of the proposals and papers submitted. As an experiment, the CeNS Innovation Award was advertised under the new name of Nano Innovation Award across the entire state of Bavaria in order to promote the prestige and visibility of the award. Many excellent proposals were submitted and total of 4 prizes were awarded.

Finally, on behalf of all CeNS members, we would like to thank the CeNS management, without whom this organization would not be possible and who have constantly shown strong commitment, great patience and energy to make things happen. Three cheers for Susanne Hennig, our managing director, Marilena Pinto, our program manager, and Claudia Leonhardt, our team assistant! I hope you will enjoy this report and find it inspiring. Long live the nano-world.



Claudia Veigel
Member of the Scientific Board of CeNS

NEW MEMBERS

DR. ULRICH LÄCHELT
LMU Munich

Ulrich Lächelt studied pharmaceutics at the University of Heidelberg, where he graduated in 2009. He joined the chair of Pharmaceutical Biotechnology at the LMU Munich and worked on his PhD thesis about multifunctional sequence-defined nucleic acid carriers under the supervision of Prof. Ernst Wagner. In 2014 he received his doctoral degree in Pharmaceutical Biology. Since then he has continued the research on drug delivery and nanomedicine as a junior research group leader and since 2017 as candidate for habilitation. His research focuses on the intracellular delivery of biomacromolecules such as nucleic acids, proteins and peptides, the development of anticancer drug conjugates and inorganic-organic hybrid materials for biomedical applications.

DR. CHRISTOF MAST
LMU Munich

Christof Mast joined the group of Prof. Dieter Braun after studying physics at LMU Munich. He was and still is fascinated by the idea of non-equilibrium physics being an essential ingredient for the emergence of life. Since then, he has focused on how thermal flows across microfluidic channels can drive even complex biomolecular reactions and how simple thermal gradients select for complex sequences, structures, and chirality.
Currently, Dr. Mast is working as a senior researcher in Prof. Braun's lab, where he is establishing novel microfluidic techniques to combine chemical and thermal non-equilibrium systems.

WELCOME BACK: PROF. THORBEN CORDES
LMU Munich

Thorben Cordes was appointed W2 professor for Physical and Synthetic Biology at the LMU Biology Department. Before, he was Associate Professor for Molecular Microscopy at the University of Groningen. Prof. Cordes has been a CeNS member since 2009.

WELCOME BACK: PROF. PHILIP TINNEFELD
LMU Munich

Philip Tinnefeld was appointed W3 professor for Physical Chemistry at the LMU Chemistry Department. He was Professor of Biophysical Chemistry at TU Braunschweig from 2010 to 2017. Prof. Tinnefeld has been a CeNS member since 2007.

NEW TO THE CENS ADVISORY BOARD: PROF. DANIEL MÜLLER

ETH Zürich, D-BSSE Basel

Prof. Daniel Müller joined the CeNS Advisory Board in January 2017. He holds the Chair of Bionanotechnology at the ETH Department of Biosystems Science and Engineering (D-BSSE) in Basel. Prof. Müller succeeds Prof. Gerd Binnig who was member of the CeNS Advisory Board from 1999 to 2017.

CALLS & APPOINTMENTS

Dr. Carsten Grashoff (MPI of Biochemistry) accepted the position of Professor for Quantitative Cell Biology at the University of Münster.

Prof. Dina Fattakhova-Rohlfing (LMU) accepted a W2 position at the University of Duisburg-Essen and as Head of Department of Electrochemical Storage, Forschungszentrum Jülich.

Dr. Stefan Wuttke (LMU) became a Senior Lecturer at the University of Lincoln (UK).

AWARDS

Prof. Thomas Carell (LMU) received an ERC Advanced Grant for his project "The Chemical Basis of RNA Epigenetics".

Prof. Wolfgang M. Heckl (TUM/ Deutsches Museum) was awarded the "Goldene Hermann-Oberth-Medaille an der Spange" for outstanding scientific and technical achievements in astronautics.

Prof. Alexander Högele (LMU) received an ERC Consolidator Grant for his project "Interfacing quantum states in carbon nanotube devices".

Prof. Ralf Jungmann (LMU/MPI of Biochemistry) became an Allen Distinguished Investigator.

Prof. Bettina Lotsch (LMU/MPI for Solid State Research) won the EU-40 Materials Prize of the European Materials Research Society.

Prof. Christian Ochsenfeld (LMU) became an Elected Board Member of the World Association of Theoretical and Computational Chemists (WATOC), Elected Member of the International Academy of Quantum Molecular Sciences (IAQMS) and Max-Planck-Fellow at MPI for Solid State Research in Stuttgart.

Dr. Alexander Urban (LMU) won an ERC Starting Grant for his research project "Perovskite Nanocrystal-Nanoreactors for Enhanced Light Emission".

Prof. Ernst Wagner (LMU) became an Academician of the European Academy of Sciences and was elected into the College of Fellows (2017) of the Controlled Release Society (CRS).

Dr. Christoph Westerhausen (Augsburg University) received an award from the Dr. Wolfbauer-Stiftung for his collaboration with the Vascular Surgery Department of the Augsburg Hospital.

CENS PUBLICATION AWARDS 2017

On November 24, the winners of the 2017 CeNS Publication Awards were announced to the CeNS members after the CeNS Annual Assembly. As is tradition, the winners were celebrated at the annual CeNS "Get-Together" event in the Café an der Universität. The awards recognized remarkably successful cooperation projects within CeNS as well as outstanding research by individual research groups from CeNS.

Best Interdisciplinary Publications:

- P. C. Nickels, B. Wunsch, P. Holzmeister, W. Bae, L. M. Kneer, D. Grohmann, **P. Tinnefeld and T. Liedl** (Science 2016, see page 41)

- F. Schüder, M. T. Strauss, D. Hörl, J. Schnitzbauer, T. Schlichthärle, S. Strauss, P. Yin, H. Harz, **H. Leonhardt and R. Jungmann** (Angew. Ch. Int. Ed. 2017, see page 64)

- Y. Tong, B. J. Bohn, E. Bladt, K. Wang, **P. Müller-Buschbaum**, S. Bals, **A. S. Urban**, **L. Poluvarapu and J. Feldmann**: From Precursor Powders to $CsPbX_3$ Perovskite Nanowires: One-Pot Synthesis, Growth Mechanism, and Oriented Self-Assembly (Angew. Ch. Int. Ed. 2017, see page 52)

Scientific Breakthrough:

- I. Vladimirov, M. Kellermeier, T. Geßner, Z. Molla, S. Grigorian, U. Pietsch, L. S. Schaffroth, M. Kühn, F. May and **R. T. Weitz** (Nano Letters 2018, see page 57)

- A. Neumann, J. Lindlau, L. Colombier, M. Nutz, S. Najmaei, J. Lou, A. D. Mohite, H. Yamaguchi and **A. Högele** (Nature Nanotechnology 2017, see page 33)

- I. R. Graf and **E. Frey** (Physical Review Letters 2017, see page 29)

- D. Saczko-Brack, E. Warchol, B. Rogez, M. Kröss, S. M. Heissler, J. R. Sellers, C. Batters, and **C. Veigel** (PNAS 2017, see page 56)

Best Junior Scientist Publication:

- L. Keil, F. Möller, M. Kieß, P. Kudella and **C. Mast** (Nature Communications 2017, see page 47)

- B. von Bronk, S. A. Schaffer, A. Götz and **M. Opitz** (PLOS Biology 2017, see page 51)

- R. Röder, T. Preiß, P. Hirschle, B. Steinborn, A. Zimpel, M. Höhn, **J. O. Rädler, T. Bein, E. Wagner, S. Wuttke and U. Lächelt** (Journal of the American Chemical Society 2017, see page 64)

- www.cens.de/research/cens-publication-award

Left: The CeNS Band "UnCenSiert " playing at the CeNS Get-Together (trumpet - Steffen Sedlak, clarinet - Hanna Engelke, piano - Martin Benoit). **Right:** Winners in the category "Best Junior Scientist Publication" Lorenz Keil and Christof Mast (from left).

FROM FUNDAMENTAL RESEARCH TO APPLICATIONS: NANO INNOVATION AWARD 2017

On July 21, 2017 the Nano Innovation Awards were awarded at CeNS. For the first time, candidates from all over Bavaria were invited to apply for the awards worth € 9,000. Three PhD students and one Master student from Würzburg and Munich won prizes for their innovative work in application-oriented nanoscience. The awardees were selected by an expert jury from industry, LMU, TUM, and the Fraunhofer Institut EMFT.

While most scientific prices emphasize findings and results in fundamental research only, the Nano Innovation Award attaches particular importance to future applicability. The prize money is donated by four successful spin-offs of CeNS, all with their own company history directly connected to the idea of the award. The companies attocube systems AG, ibidi GmbH, Nanion Technologies GmbH, and NanoTemper Technologies GmbH, together with CeNS honor gifted and creative junior researchers, whose results are not only interesting for fundamental research but also promising for technological applications.

Physicist Florian Schüder from the group of Professor Ralf Jungmann (MPI of Biochemistry/ LMU München) received an award worth € 3,000 in the category "Master's thesis". Super-resolution techniques are starting to revolutionize biology by enabling researchers to observe structures inside cells with unprecedented spatial resolution, beating the classical diffraction limit by more than an order of magnitude. However, most techniques are restricted for technical reasons to structures that are very close to the cover glass, thus preventing whole-cell or tissue imaging with standard instrumentation. In his master's thesis research, Florian Schüder implemented the recently developed DNA-PAINT super-resolution technique using a minimally modified spinning-disk confocal microscope to extend imaging to whole cells and potentially tissues. Due to the wide availability of spinning-disk microscopes in standard biology labs and imaging facilities, researchers can now answer questions with super-resolution in whole cells and beyond.

In the category "PhD thesis", the jury split the prize worth € 6,000 among three awardees:

Magnetic Particle Imaging (MPI) is a new tomographic imaging method for the 3D-detection of superparamagnetic iron-oxide nanoparticles (SPIONs). In the thesis work of **Dr. Patrick Vogel (group of Professor Peter Jakob, Julius-Maximilians-Universität Würzburg)**, a novel scanner concept, the traveling wave MPI (TWMPI) system, which allows the rapid and highly sensitive visualization of SPIONs, was developed and built. TWMPI is a promising non-invasive imaging modality that has already been able to prove its great potential for the fields of medicine, biology and geology in preliminary experiments.

For more than 60 years cytostatic agents have been used in chemotherapy against cancer but have featured no selectivity exclusively for cancer cells. Most of these cytostatics also affect the healthy tissue of the human body, causing lasting harm and severe side effects. The PhD thesis of the chemist **Dr. Stefan Datz (group of Professor Thomas Bein, LMU München)** focused on the synthesis and modification of nanomaterials for drug delivery applications to specifically target cancerous tissue without harming healthy tissue. The requirements for efficient stimuli-responsive and thus controllable release of cargo molecules into cancer cells and the design principles for smart and autonomous nanocarriers are discussed in the thesis.

From left to right: Nano Innovation Award winners Dr. Peter Röttgermann, Dr. Patrick Vogel, Florian Schüder, and Dr. Stefan Datz.

Personalized medicine is going to be the main achievement of patient care. Under the motto "One patient, one tumor profile, one personalized treatment" a novel micropatterning technique was developed in the scope of **Dr. Peter Röttgermann's PhD thesis (group of Professor Joachim Rädler, LMU München)**. These micropatterns allow thousands of single cells to be screened in parallel for different cell death markers in a time-resolved way. Analysis of these heterogeneous multi-color signals identifies the right compound of drugs for successful tumor treatment.

■ www.cens.de/research/nano-innovation-award

CENS TRAVEL AWARDS

In 2017, fourteen CeNS PhD students and three postdocs won CeNS travel awards to present their work at international conferences and workshops. The recipients of the awards came from thirteen different CeNS groups, from the Department of Chemistry, the Department of Physics and the Faculty of Medicine. 47% of the awardees were female. The CeNS travel award comes with up to €1,500 for travel costs.

■ **Sidney Becker** (AG Carell): XVIIIth International Conference on the Origin of Life, San Diego
■ **Linda Brützel** (AG Lipfert): European Biophysical Conference 2017, Edinburgh
■ **Irene Grill** (AG Hartschuh): 2017 MRS Fall Meeting, Boston
■ **Franziska Kriegel** (AG Lipfert): European Biophysical Conference 2017, Edinburgh
■ **Claudia Lermer** (AG Lotsch): ACS Spring Meeting, San Francisco
■ **Christoph Maier** (AG Feldmann): 2017 MRS Fall Meeting, Boston
■ **Aurora Manzi** (AG Feldmann): 2017 MRS Fall Meeting, Boston
■ **Matthias Morasch** (AG Braun): XVIIIth International Conference on the Origin of Life, San Diego
■ **Alexandra Murschhauser** (AG Rädler): 62nd Annual Meeting Biophysical Society, San Francisco
■ **Wolfgang Ott** (AG Gaub): European Biophysical Conference 2017, Edinburgh
■ **Michiel Petrius** (AG Bein): International Conference on Hybrid and Organic Photovoltaics (HOPV 17), Lausanne
■ **Mauricio Pilo-Pais** (AG Liedl): APS March Meeting, New Orleans
■ **Petra Rovo** (AG Linser): 10th Alpine Conference on Solid-State NMR, Chamonix
■ **Dario Sazcko-Brack** (AG Veigel): DPG Frühjahrstagung, Dresden
■ **Florian Schüder** (AG Jungmann): Focus on Microscopy, Singapur
■ **Yinghong Hu** (AG Bein): Perovskite Solar Cells and Optoelectronics (PSCO) conference 2017, Oxford
■ **Thomas Zettl** (AG Lipfert): Biophysical Society 61th Annual Meeting, New Orleans

■ www.cens.de/research/nano-innovation-award

SPIN-OFF NEWS

ATTOCUBE

Not only precise, but also beautiful: The Ultra Precision Sensor IDS3010 received the iF Design Award 2017. The award is given for exceptional design and considered to be one of the most important design prizes in the world.
Moreover, attocube celebrated the roofing ceremony of their new headquarters in Haar close to Munich on September 8, 2017. The company with its 100 employees will move there together with their affiliated company neaspec GmbH & WITTENSTEIN alpha next year.
■ www.attocube.com

From left to right: Dr. Max Scheible, Prof. Philip Tinnefeld, Dr. Jürgen Schmied, and Dr. Carsten Forthmann from Gattaquant, winners of the Technology Transfer Awad of the IHK Braunschweig.

ETHRIS

Ethris has started a five-year cooperation with AstraZeneca to further develop mRNA therapies, receiving an advance payment of €25 million in the process. The new license agreement underlines Ethris' leading position in mRNA therapies. "This cooperation connects our proprietary technology with AstraZeneca's and MedImmune's world-class expertise in respiratory diseases, the development of biologicals, and commercialisation," says Carsten Rudolph, CEO of Ethris.
■ ethris.com

GATTAQUANT

GATTAquant GmbH is a spin-off company from the group of Prof. Philip Tinnefeld in the field of super-resolution imaging. The company focuses on probes for fast, easy, and precise quantification of super-resolution systems. In 2017, Gattaquant was the proud winner of the Technology Transfer Award of the IHK Braunschweig, worth €10,000.
■ www.gattaquant.com

GNA BIOSOLUTIONS

In 2017, GNA Biosolutions launched the Pharos V8, the world's first laser PCR® platform. Pharos V8 is an ultrafast PCR instrument for in vitro research use. Laser PCR® operates on the same principles as conventional nucleic acid amplification with PCR, but uses nanomaterials to control temperature cycles at the nano scale, accelerating PCR reaction times by a factor of ten and opening the door for applications in multiple time-sensitive settings.
The Pharos V8 is the company's first platform to come on the market, with additional product launches planned over the next two years.
■ www.gna-bio.de

NANION TECHNOLOGIES

Nanion Technologies announced the launch of the new SURFE2R 96SE Instrument for high throughput measurements of electrogenic membrane transporters and pumps. The SURFE2R 96SE is the first instrument on the market featuring the solid supported membrane (SSM) technology for robust and simple screening of membrane transporters and pumps in a high throughput manner. In this way, the SURFE2R 96SE opens up new perspectives in membrane protein screening and investigations for the pharmaceutical industry, offering label- and radioactivity-free analysis for these difficult targets.
Nanion Technologies' Munich headquarters moved to new and larger facilities in Ganghoferstraße close to the city center in May 2017. Dr. Niels Fertig says: "We found the ideal space within the former laboratories of Daiichi Sankyo Germany and we are very pleased with the new site - a modern building which meets our requirements in terms of technical infrastructure and laboratory facilities."

■ www.nanion.de

CeNS company visit: CeNS students and Dr. Niels Fertig on the roof terrace of Nanion's new headquarter in Ganghoferstraße.

NANOTEMPER TECHNOLOGIES

NanoTemper Technologies won the "Innovators of the Year 2017" prize in the Top 100 competition, the award for Germany's most innovative SMEs. The company was selected as the winner in category B (51-100 employees).

■ www.nanotemper.de

Innovators of the Year 2017 (From left to right): TOP 100 mentor Ranga Yogeshwar, Dr. Stefan Duhr and Dr. Philipp Baaske (NanoTemper Technologies GmbH), and Prof. Dr. Nikolaus Franke, scientific head of TOP 100. Image Copyright: KD Busch/compamedia.

SPIN-OFF PORTRAIT

GNA BIOSOLUTIONS

The GNA Biosolutions team.

"Beyond molecular boundaries"- this is GNA Biosolutions' slogan. The company, a spin-off from the LMU Faculty of Physics, was founded by Dr. Federico Bürsgens and Dr. Joachim Stehr, two former PhD students from the group of Professor Jochen Feldmann, and Dr. Lars Ullerich, a former PhD student at the Institute for Innovation Research, Technology Management and Entrepreneurship at LMU. Located in the IZB (Innovations- und Gründerzentrum) in Martinsried, GNA develops instruments, OEM modules, and ultrafast molecular tests. Last year, the company launched the Pharos V8, an ultrafast laser PCR instrument.

How and when was GNA Biosolutions founded?

GNA was founded as a company in 2010. We were a spin-off from the Chair for Photonics and Optoelectronics (Professor Feldmann).

What role did the university play in the foundation of GNA Biosolutions?

We were supported by LMU's Spin-off Service and the Entrepreneurship Center. Furthermore, we were able to maintain a fruitful collaboration with the chair.

What product does GNA Biosolutions sell and what are its main features?

GNA recently launched the Pharos V8, an ultrafast laser PCR instrument designed for time-sensitive molecular applications. With laser PCR technology, nucleic acid amplification can be performed up to 10 times faster than with conventional methods

What were your biggest challenges along the way?

In the beginning we focused on developing our core technology platform, which took several years. We needed to stay focused on our core offering, our technology platform, while still

The Pharos V8, an ultrafast Laser PCR instrument.

raising funds to grow the company. We also needed to stay flexible enough to adjust our business plan as our technology matured.

How many employees work for GNA Biosolutions today?
GNA Biosolutions now has a team of 30 scientists, engineers and application specialists.

How important are the contacts to academic institutions like CeNS for you?
Our roots are in academia, so this is the culture we come from, and we value the opportunity to be in contact with experts and research talents.

How did you acquire the necessary entrepreneurial knowledge to found and run a company?
One of our founders graduated in innovation management at LMU, so entrepreneurship knowledge was a core competency within our founding team. When we first started out it was also important to get external feedback, so we participated in business plan competitions, which was very valuable. The most important thing we did was to just learn by doing, be very hands-on, and open to continuously learning new skills.

What are your major goals for the future?
Today molecular testing is still a specialist field and is done mainly in laboratories. Our vision is to use our technology to take molecular testing out of the lab and bring it to as many applications and setting as possible - we want molecular testing to be something that happens in the real world, not just at the bench. Right now, we are developing a device that will be able to analyze pathogens in 15 minutes from sample to result.

What would be your most important advice for researchers on their way to becoming an entrepreneur?
Learn and listen, stay focused, and keep moving forward.

Answers by Dr. Lars Ullerich.

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EVENTS & ACTIVITIES

CENS/SFB1032 WORKSHOP VENICE

"Design and control of nanosystems" - this was the motto of the annual CeNS workshop in 2017 at Venice International University / San Servolo. The workshop was a joint effort with the Collaborative Research Centre SFB1032 "Nanoagents for the spatiotemporal control of molecular and cellular reactions". The program committee, Thomas Carell, Erwin Frey, Don Lamb, Hubert Krenner, and Ulrich Schollwöck, drew up an impressive schedule with renowned speakers from all over the world (Aleksei Aksimentiev, Julie Biteen, Alex Deiters, Jörn Dunkel, Nikta Fakhri, Nigel Goldenfeld, Peter Hommelhoff, Klaus Kroy, Christoph Lienau, L. Mahadevan, Laurens Molenkamp, Daniel Müller, Rob Phillips, Mikael Rechtsman, Gil Refael, Sanford Simon, Michael Strano, Ronny Thomale, Rinaldo Trotta), covering a wide range of topics from bionanoscience, nanomaterials, optoeletronics and hybrid technologies to quantum phenomena. In addition, senior and junior researchers from the Munich area (Frank Pollmann, Oliver Trapp, Ivan Huc, Christoph Westerhausen, and Peter Röttgermann) provided insights into their work.
A special highlight was the two keynote talks on future challenges in biophysics by Rob Phillips and on the quantum revolution by Gil Refael.
PhD students and master's students, including Junior Nanotech Network participants from Munich and the University of Illinois at Urbana-Champaign, presented and held a lively discussion of their latest results during the two poster sessions.

■ www.cens.de/calendar/workshops-events/venice-2017

CENS MEETS INDUSTRY

As every year, CeNS invited representatives and alumni from various business sectors to present their company and employment opportunities to the junior researchers of CeNS. In 2017, CeNS had organized a very diverse program with representatives from the Fraunhofer Gesellschaft, Google Inc., the CeNS spin-off GNA Biosolutions GmbH, and CeNS alumni working in large companies such as Linde AG, TOPTICA Photonics AG, and Siltronic AG. The event was followed by the traditional CeNS summer party in the Salinenhof, where the CeNS band "UnCeNSiert" infected the guests with good vibrations. A highlight was the presentation of the Nano Innovation Award winners (see page 10). As always, the summer party was a great opportunity for discussions between CeNS members, speakers, guests, and alumni.

■ www.cens.de/calendar/past-workshops-events/cens-meets-industry-2017

KEY QUALIFICATION WORKSHOPS

CeNS supported its associates with several key qualification workshops. A workshop on scientific publishing and the Nature journal family was organized together with the CeNS alumnus Dr. Kyle Legate in May 2017. To help them acquire the skills necessary for successful scientific presentations and publications, students had the opportunity to attend two workshops, which introduced them to the principles of effective visual communication and the design of scientific illustrations. In addition, CeNS associates took the chance to join the three-day Entrepreneurship Seminars organized by the LMU Entrepreneurship Center.

■ www.cens.de/calendar/past-workshops-events

MUNICH SCIENCE DAYS

The 17th Munich Science Days (November 25 – 28, 2017) dealt with the subject "Plans for the Future: Research, Society, People". Together with the Nanosystems Initiative Munich, CeNS presented the topic "Shaping the future with Nano" to the public over the four days. PhD students and group leaders from the CeNS/NIM groups of Thomas Bein, Hermann Gaub, Bettina Lotsch, and Ernst Wagner presented research projects on nanomaterials for energy conversion or drug delivery systems for new applications in nanomedicine. Nano-experiments for kids, a tabletop football game illustrating drug delivery, interesting exhibits like an AFM model, a nano quiz and most of all the enthusiasm of the junior researchers when explaining their projects made the CeNS/NIM booth a center of attraction for visitors.

■ www.muenchner-wissenschaftstage.de/rueckblick-2017

CENS COMPANY VISITS

Due to the great success of the visits in the previous year, CeNS again organized two on-site company visits. In July 2017, a student group had the unique chance to visit Nanion Technologies' brand-new R&D and production site in Ganghoferstraße. Niels Fertig, founder and CEO of Nanion and a CeNS member, provided fascinating insights into Nanion's history, product lines, and visions. In addition, the students had the chance to discuss future career and business opportunities.
The second company visit was to Roche Penzberg, a global player located in the Munich area. The 15 participants were informed about early development in diagnostic research, met CeNS alumni Dr. Susanne Seidel and Dr. Peter Röttgermann, and learned about career opportunities for physicists and chemists.

■ www.cens.de/calendar/past-workshops-events

RESPONSIBLE RESEARCH

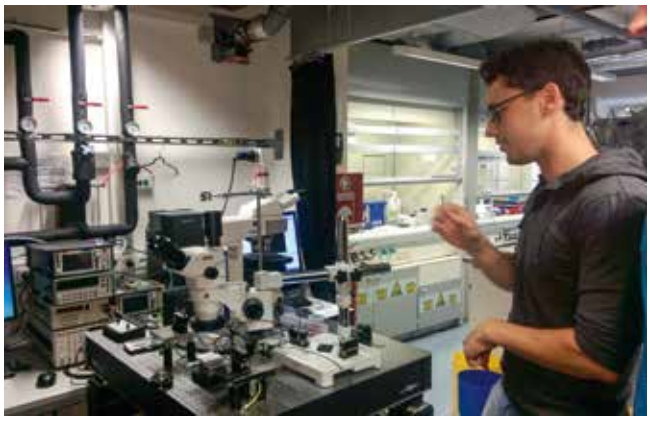
In 2017, seventeen graduate programs from the Life Science Campus Großhadern/Martinsried, the GraduateCenter LMU, and CeNS jointly hosted an event on responsible research conduct. Plagiarism, data reproducibility, image integrity, open science, and the German ombudsman system were the topics adressed for next generation researchers in keynote lectures, e.g., by DFG Ombudsperson Professor Dr. Joachim Heberle, and breakout sessions. In addition, a web-based "toolbox" providing additional information about good scientific practice was established and is available online.

■ www.responsibleresearch.graduatecenter.lmu.de

CENS LAB TOUR

The CeNS 2017 lab tour, organized by the student representatives, took place at the Faculty for Physics. The participants were guided through the labs of Prof. Weitz, Prof. Bloch, and Prof. Rädler by peer PhD students. They learned about research and infrastructure such as charge transport in organic semiconductors, quantum many body systems, and microstructured environments for collective cell migration. The tour was followed by a barbecue on the physics roof terrace organized by the students, a perfect opportunity to meet people from different CeNS groups and to exchange ideas.

- www.cens.de/calendar/past-workshops-events



CENS B2RUN

For the first time, a CeNS team entered the B2Run-company competition in Munich. PhD students, postdocs, one CeNS professor, technical and administrative staff joined the "CeNSation" team and all made it to the finishing line after running 6.1 km through the Olympic Park.

PATENTS - HOW TO PROTECT YOUR IDEAS

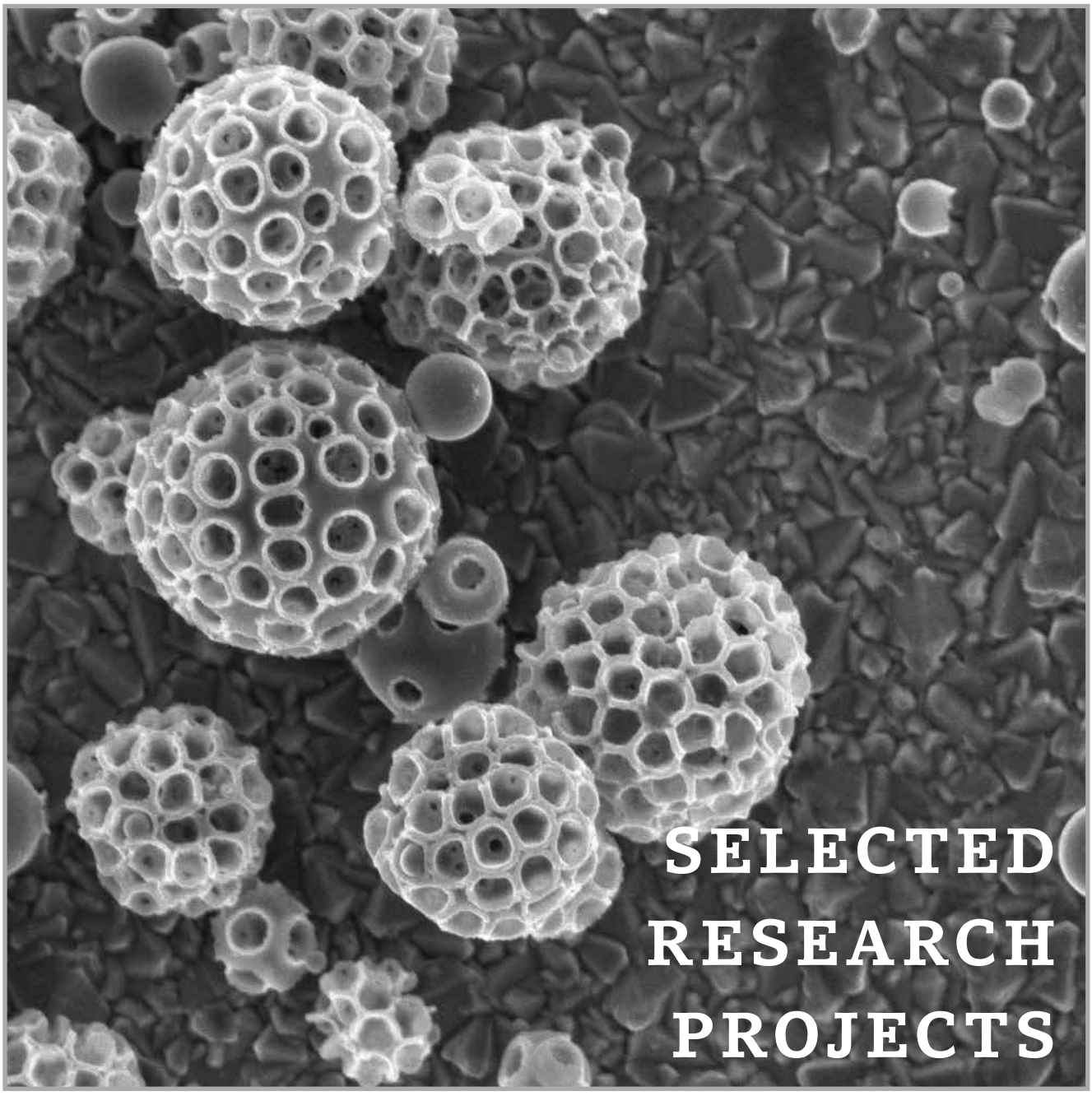
On March 27 and 28, 2017, CeNS organized a workshop on intellectual property and patent protection for 29 postdocs and PhD students from CeNS and related programs. Patent attorney Dr. Stefan Huebner started with a presentation on how to protect nanotechnology inventions successfully, introducing the most fundamental aspects of IP law. Dr. Sarah Krüger, Bayerische Patentallianz GmbH, continued with a talk about IP protection at universities, and management and commercialization strategies by the BayPat. The third talk by CeNS alumnus Dr. Christian Kallinger (EPO) addressed the patenting procedure at the European Patent Office. The afternoon ended with a fireside chat about career opportunities in the IP sector. On the second day, the participants put themselves into the roles of patent attorneys and judges. They worked in groups on a real patent infringement case and then presented their arguments in a mock trial.

- www.cens.de/calendar/past-workshops-events

JUNIOR NANOTECH NETWORK

The seventh Junior Nanotech Network exchange (JNN) was organized jointly with the Center for the Physics of Living Cells (CPLC) at the University of Illinois at Urbana-Champaign. Initiated by CeNS member Prof. Jan Lipfert together with Prof. Aleksei Aksimentiev and Prof. Zan Luthey-Schulten from Illinois, four PhD students from the CPLC travelled to Munich for the first part of the exchange from September 11-24, 2017. The guests were hosted by CeNS PhD students from the groups of Dieter Braun, Anna Cattani-Scholz, Tim Liedl, Rasmus Linser, Joachim Rädler, Petra Schwille and Christoph Westerhausen.
The participants did one week of lab rotations, performing hands-on experiments at LMU, the MPI of Biochemistry and Augsburg University, taught by their peer students from CeNS. Topics ranged from DNA origami and NMR spectroscopy of biological supra-molecules to microfluidic channels for thermodynamical and mechanical modulation of transmembrane transport on living cells. The lab work was complemented by the CeNS workshop in Venice, where the JNN participants presented posters and networked with the CeNS community and invited speakers.
Besides the scientific program, the visit was filled with social activities that brought the participants closer to German culture and history, such as a tour of historic Augsburg, an meal at a typical Bavarian restaurant, and a visit to the opening day of the Oktoberfest.

- www.cens.de/international/exchange-programs/jnn



SELECTED RESEARCH PROJECTS

1

DIRECTIONAL CHARGE-CARRIER TRANSPORT IN ORIENTED BENZODITHIOPHENE COVALENT ORGANIC FRAMEWORK THIN FILMS

Prof. Thomas Bein (LMU München, Chemistry Department) ■ bein.cup.uni-muenchen.de

Charge-carrier transport in oriented Covalent Organic Framework (COF) thin films is an important factor for realizing COF-based optoelectronic devices. The group of Thomas Bein describes how highly oriented electron-donating benzodithiophene BDT-COF thin films serve as a model system for a directed charge-transport study. Oriented BDT-COF films were deposited on different electrodes with excellent control over film roughness and structure, allowing for high-quality electrode COF interfaces suitable for device fabrication. Hole-only devices were constructed to study the columnar hole mobility of the BDT-COF films. The transport measurements reveal a clear dependency of the measured hole mobilities on the BDT-COF film thickness, where thinner films showed about two orders of magnitude higher mobilities than thicker ones. Transport measurements under illumination yielded an order of magnitude higher mobility than in the dark. In-plane electrical conductivity values of up to 5 x 10^{-7} S/cm were obtained for the oriented films. Impedance measurements of the hole-only devices provided further electrical description of the oriented BDT-COF films in terms of capacitance, recombination resistance, and dielectric constant. An exceptionally low dielectric constant value of approximately 1.7 was estimated for the BDT-COF films, a further indication of their highly porous nature. DFT and molecular-dynamics simulations were carried out to gain further insights into the relationships between the COF layer interactions, electronic structure, and the potential device performance.

■ **D. D. Medina, M. L. Petrus, A. N. Jumabekov, J. T. Margraf, S. Weinberger, J. M. Rotter, T. Clark, and T. Bein:** *Directional Charge-Carrier Transport in Oriented Benzodithiophene Covalent Organic Framework Thin Films;* ACS Nano 11 (3), 2706-2713 (2017).

Fig.1: Scheme showing oriented boronic ester-based benzodithiophene covalent organic framework thin film sandwiched between electrodes for measurement of charge migration behavior. Illustration: Christoph Hohmann, NIM.

2

BIOPHYSICAL APPROACHES TO ASSESS THE FUNCTION OF VON WILLEBRAND FACTOR - AN ESSENTIAL BLOOD CLOTTING MOLECULE

Martin Benoit (LMU Munich, Faculty of Physics)
Joachim Rädler (LMU Munich, Faculty of Physics)

- www.biophysik.physik.lmu.de
- www.softmatter.physik.lmu.de

The process of hemostatic plug formation at sites of vascular injury crucially relies on the large multimeric plasma glycoprotein von Willebrand factor (VWF) and its ability to recruit platelets to the damaged vessel wall. Under normal blood flow conditions, VWF multimers hardly interact with platelets to maintain the blood flow. Only when subjected to increased hydrodynamic forces, which primarily occur in connection with vascular injury, VWF can efficiently bind to platelets. VWF multimers respond to elevated hydrodynamic forces by elongation, thereby reversibly increasing their adhesiveness to platelets. Thus, the activation of VWF is force-induced, as is its inactivation. This force-regulation of VWF's hemostatic activity is not only highly intriguing from a biophysical perspective, but also of eminent physiological importance. AFM imaging and in particular AFM force spectroscopy efficiently uncover structural and mechanical information on VWF oligomers. Within a strong interdisciplinary and international VWF-research network, complementary biophysical, biochemical and medical methods are combined to gain novel insights into the multiple aspects of VWF.

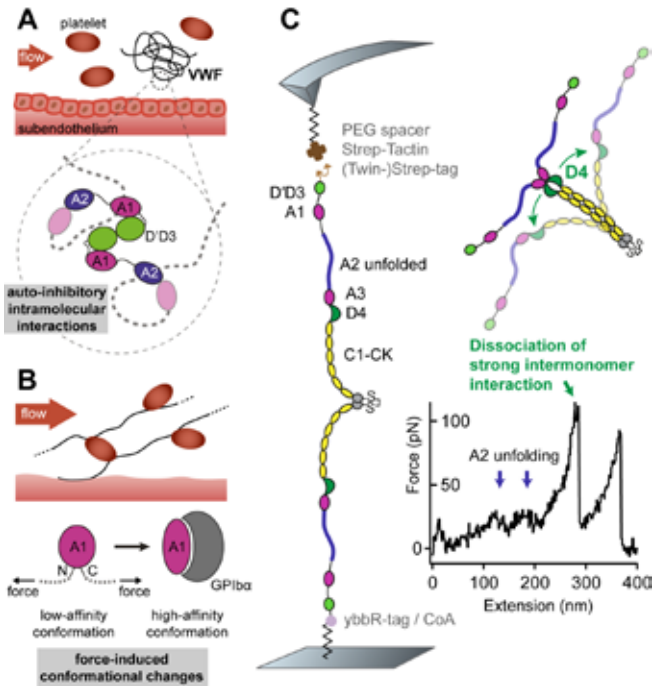


Fig. 1: Large VWF multimers freely circulate in the blood stream in an inactive conformation (A). Upon elevated shear forces occurring at sites of injury VWF is activated both by removal of auto-inhibitory intramolecular interactions and by local conformational changes, resulting in increased platelet binding (B) via the A1 domain. (C) By AFM force spectroscopy, force-induced conformational changes can be studied at the single-molecule level to gain insights into the relation between force, structure and function.

- **A. Löf, J.P. Müller, M. Benoit, M.A. Brehm:** *Biophysical approaches promote advances in the understanding of von Willebrand factor processing and function;* Advances in Biological Regulation 63, 81-91 (2017).

A. Löf, J.P. Müller, and M.A. Brehm: *A Biophysical View on von Willebrand Factor Activation*; Journal of Cellular Physiology, doi: 10.1002/jcp.25887 (2017).

3

FROM DETECTING STROKE RISKS WITH NANOTEMPER TO UNRAVELING REPLICATION MODES OF THE EMERGENCE OF LIFE

Prof. Dieter Braun (LMU München, Physics Department) ■ www.biosystems.physik.lmu.de

The Braun lab could, with the help of NanoTemper Technologies, perfect techniques to measure delicate elastase proteins in patients' blood serum. In a large collaboration, they could help in finding a functionally relevant coding sequence variation, which confers the risk for large artery atherosclerotic stroke. They could show that the single-residue variation M1(A213V) in serpin family from Ala-to-Val altered its functional dynamics toward neutrophil elastase in the presence of complex lipid-containing plasma and also affects the overall structural flexibility of the protein.

To study the possibilities for the first living molecules on early Earth to survive, the Braun lab implemented pH gradients across rock membranes. One theory for the origin of life proposes that geological pH gradients were the prebiotic ancestors of these cellular disequilibria. The existence of 6 pH-unit gradients was shown across micrometer scales in a microfluidic vent replicates. Precipitation of metal sulfides at the interface strengthened the gradients and sustained the disequilibria in the absence of flow. The results confirmed that alkaline vents can provide an exploitable pH gradient, supporting their potential role at the emergence of chemiosmosis and the origin of life.

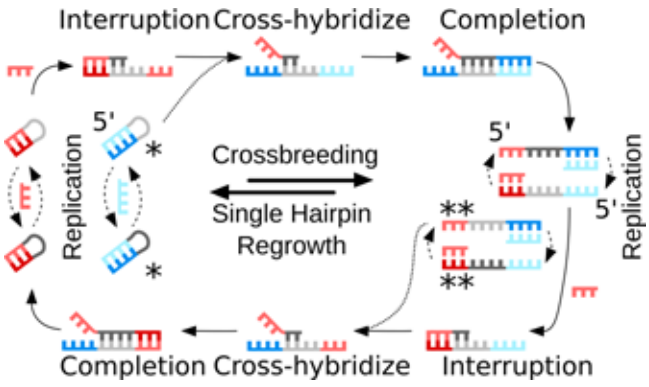


Fig. 1: Replicators of DNA can form two phenotypes. Either they replicate slow as a hairpin, but then only require one replicator binding site. Or two of these hairpin replicators recombine and form a fast replicating mutant, but now requires two replicator binding sites. Depending on the environment, the replicating sequence can switch between both forms.

Especially the role of early replication mechanisms were essential for the emergence of life. How could molecules with short lifetimes preserve their information over millions of years? For evolution to occur, information-carrying molecules have to replicate before they degrade. The Braun lab revealed by experiment a robust, reversible cooperation mechanism in oligonucleotide replication. Two inherently slow replicating hairpin molecules could transfer their information to fast crossbreed replicators that outgrow the hairpins. The reverse was also possible. With this mechanism, interacting replicators can switch between the hairpin and crossbreed mode, revealing a flexible adaptation to different boundary conditions.

■ **Rainer Malika, Therese Daub, Maria Gonik, Anirudh Sivakumar, Daniel J. Deredge, Evgeniia V. Edeleva, ...,Dieter Braun, Hugh S. Markus, Patrick L. Wintrode, Klaus Berger, Dieter E. Jenne, and Martin Dichgans:** *Common coding variant in SERPINA1 increases the risk for large artery stroke;* PNAS, doi: 10.1073/pnas.1616301114 (2017).

Georg C. Urtel, Thomas Rind and Dieter Braun: *Reversible Switching of Cooperating Replicators;* Phys. Rev. Lett. 118, 078102, doi: 10.1103/PhysRevLett.118.078102 (2017).

Friederike M. Möller, Franziska Kriegel, Michael Kieß, Victor Sojo and Dieter Braun: *Steep pH Gradients and Directed Colloid Transport in a Microfluidic Alcaline Hydrothermal Pore;* Angew. Chem., doi: 10.1002/anie.201610781R2; (2017).

4

FINDING A NEEDLE IN A HAYSTACK / DENDRIMER-BASED SIGNAL AMPLIFICATION FOR DETECTING PROLIFERATING CELLS

Prof. Thomas Carell (LMU Munich, Department of Chemistry) ■ www.carellgroup.de
Prof. Christoph Bräuchle (LMU Munich, Department of Chemistry) ■ www.cup.lmu.de/pc/braeuchle
Dr. Hanna Engelke (LMU Munich, Department of Chemistry) ■ www.cup.lmu.de/pc/engelke

Finding a needle in a haystack: The proliferation rate of cells is a key parameter, e.g. in cancer diagnostics, where it is required to measure the proliferation of cells with high precision, even down to single cancer cells, in a patient sample. A new method to detect proliferating cells *in situ* by using multiple consecutive click reactions with dendrimeric molecules and clickable dyes is presented in the publication cited below. These assays have outstanding sensitivities. Signal intensities and signal-to-noise ratios are far better than those obtained by techniques that are currently available.

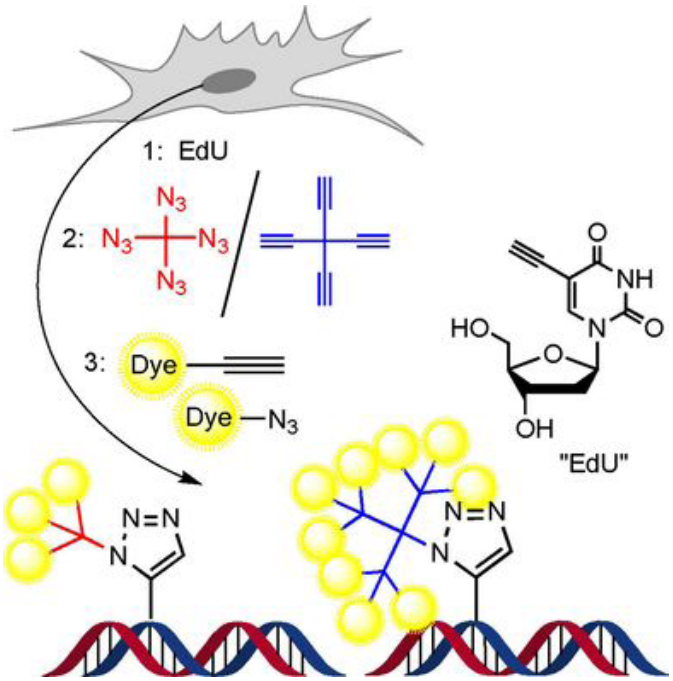


Fig. 1: Dendrimer organization and consecutive click reactions in the diagnostic assays.

■ **N. Raddaoui*, S. Stazzoni*, L. Möckl, B. Viverge, F. Geiger, H. Engelke, C. Bräuchle, T. Carell*:** *Dendrimer-Based Signal Amplification of Click-Labelled DNA in Situ;* ChemBioChem 18, 1716 (2017).

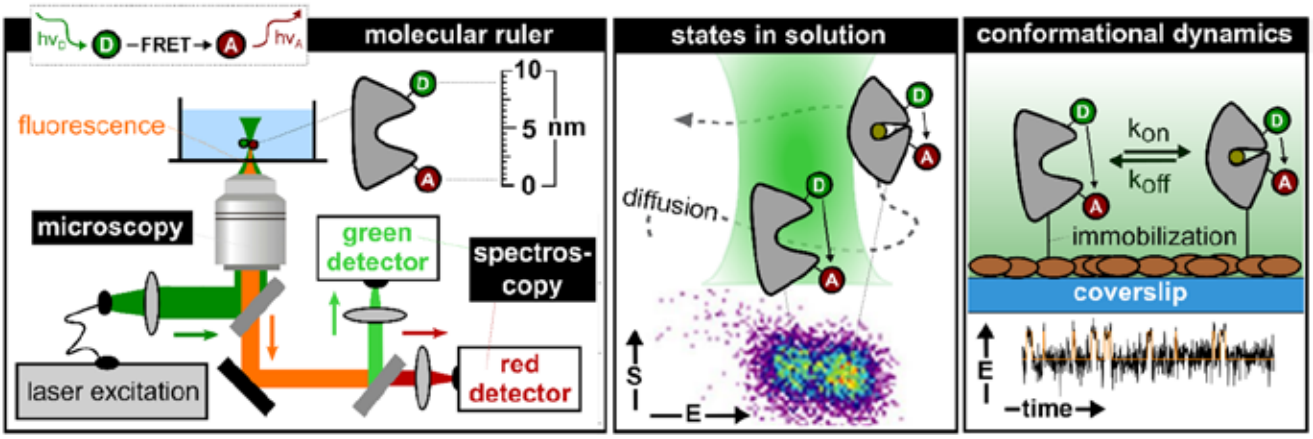
5

FROM QUALITATIVE ASSESSMENT OF CONFORMATIONAL STATES TOWARDS QUANTITATIVE DISTANCES TO UNDERSTAND LIGAND REJECTION IN MEMBRANE TRANSPORTERS

Prof. Thorben Cordes (LMU Munich, Faculty of Biology)
- www.mikrobiologie.biologie.lmu.de/forschung/ag_cordes/index.html

Prof. Jan Lipfert (LMU Munich, Department of Physics)
- www.molecularbiophysics.physik.lmu.de

The Cordes lab started to monitor conformational states of bacterial ABC transporters via biophysical measurements to unravel molecular principles, transport kinetics and with this to establish a direct structure-function relationship. The biophysical approach relies on determination of Förster-resonance energy transfer efficiency, which can be used as an indicator for conformational states. In such an experiment a single restrained distance is related via structural analysis to distinct biochemical states. The major obstacle in quantitative FRET-spectroscopy is to relate FRET efficiency distributions to accurate distances or –ideally– full distance distributions that reflect the underlying molecular ensemble. Recent work from the Lipfert lab has demonstrated a novel approach to measure molecular distances, based on attaching pairs of small (~1 nm) gold labels to biological macromolecules. The gold-gold distances are read out using anomalous small-angle X-ray scattering. The novel method anomalous scattering interference (AXSI) overcomes several limitations of FRET: AXSI i) directly measures absolute distances, ii) obtains the full distribution of distance of the molecular ensemble in solution, and iii) can resolve distances >10 nm.
The proposed collaborative project aims at a quantitative validation of FRET-based distance measurements via a correlation of FRET data with the new anomalous X-ray scattering interference (AXSI) method. The quantitative information available from AXSI is essential to understand the involvement of different conformational states of SBDs as an element of discrimination between correct and incorrect ligands, where the latter are known not to be transported. In addition, the work would provide a proof-of-concept for the applicability of the AXSI to detect conformational changes in a complex protein ensembles.



6

LIPID-COATED METAL-ORGANIC FRAMEWORK NANOPARTICLES: AN EFFICIENT DRUG DELIVERY PLATFORM

Hanna Engelke (LMU Munich, Department of Chemistry) ■ www.cup.lmu.de/pc/engelke/
Stefan Wuttke (LMU Munich, Department of Chemistry) ■ www.wuttkegroup.de

This collaboration between the groups of Stefan Wuttke and Hanna Engelke resulted in the development of a drug delivery system based on metal-organic framework (MOF) nanoparticles encapsulated in exosomes that synergistically combines the favorable properties of both materials. Exosomes are lipid vesicles produced by cells for information transport purposes and they can deliver cargo without being attacked by the immune system. In the future they can be directly derived from the patient and pave the way toward personalized medicine. MOF nanoparticles are highly tunable in their chemical and physicochemical properties, offer high loading capacities, and thus are considered a highly promising nanocarrier material. Neither exosomes nor MOF nanoparticles by themselves can perform efficient drug delivery without premature leakage.
However, the combination of MOF nanoparticles and exosomes as coating allows for the creation of an efficient and flexible delivery platform for biologically active molecules. For this purpose, lipid fusion was employed to coat the MOF nanoparticles with exosomes and encapsulate cargo molecules non-covalently. The resulting exosome-coated MOF nanoparticles are taken up by cells and efficiently release their cargo without premature release. A potential application in chemotherapy was demonstrated by successful delivery of the chemotherapeutic agent SBHA to cancer cells in vitro that results in significantly reduced cell viability. With a similar system successful delivery of a combination of two chemotherapeutics could be achieved paving the way for combination therapy in the fight against resistances. The underlying novel release mechanism is most likely based on the decomposition of the MOF nanocarrier creating osmotic pressure in the endosome that allows for rupture of the endosomal membrane followed by release of the cargo carried by the MOF nanoparticle.

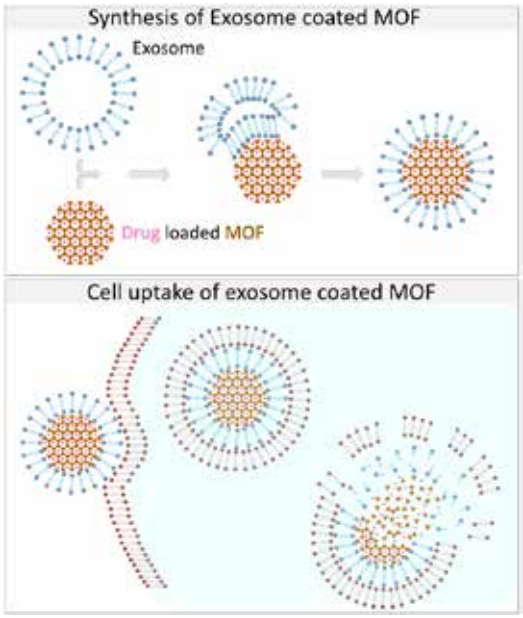


Fig. 1: Schematic illustration of the synthesis of the exosome coated MOF and the subsequent cell uptake and proposed release mechanism of the cargo. Reprinted with permission from Illes et al. Chemistry of Materials, 29, 8042–804 (2017), Copyright 2018 American Chemical Society.

The advantages of both exosomes and MOF nanoparticles could only be appreciated in this combination of the two materials providing a versatile platform for future research on drug delivery.

■ **B. Illes, P. Hirschle, S. Barnert, V. Cauda, S. Wuttke, and H. Engelke:** *Exosome-coated Metal-Organic Framework Nanoparticles: An Efficient Drug Delivery Platform;* Chemistry of Materials, 29, 8042–804 (2017).

B. Illes, S. Wuttke, H. Engelke: *Liposome-Coated Iron Fumarate Metal-Organic Framework Nanoparticles for Combination Therapy;* Nanomaterials, 7, 351 (2017).

7

ROCK SALT NI/CO OXIDES WITH UNUSUAL NANOSCALE-STABILIZED COMPOSITION AS WATER SPLITTING ELECTROCATALYSTS

Prof. Dina Fattakhova-Rohlfing (Forschungszentrum Jülich)
- www.fz-juelich.de/iek/iek-1/DE/Forschung/ElektrochemischeSpeicher

Prof. Thomas Bein (LMU München, Chemistry Department)
- bein.cup.uni-muenchen.de

The influence of nanoscale on the formation of metastable phases is an important aspect of nanostructuring that can lead to the discovery of unusual material compositions. The groups of Dina Fattakhova-Rohlfing and Thomas Bein have investigated the synthesis, structural characterization, and the electrochemical performance of Ni/Co mixed oxide nanocrystals in the hydrogen evolution reaction (HER) and oxygen evolution reaction (OER), with a focus on the influence of nanoscaling on their composition and solubility range. Using a solvothermal synthesis in tert-butanol, they obtained ultrasmall crystalline and highly dispersible $Ni_xCo_{1-x}O$ nanoparticles with rock salt type structure. The mixed oxides feature non-equilibrium phases with unusual miscibility in the whole composition range, which is attributed to a stabilizing effect of the nanoscale combined with kinetic control of particle formation. Substitutional incorporation of Co and Ni atoms into the rock salt lattice has a remarkable effect on the formal potentials of NiO oxidation that shift continuously to lower values with increasing Co content. This can be related to a monotonic reduction of the work function of (001) and (111)-oriented surfaces with an increase in Co content, as obtained from density functional theory (DFT+U) calculations. Furthermore, the electrocatalytic performance of the $Ni_xCo_{1-x}O$ nanoparticles in water splitting changes significantly. OER activity continuously increases with increasing Ni content, while the HER activity shows the opposite trend, increasing for higher Co contents. The high electrocatalytic activity and tunable performance of the nonequilibrium $Ni_xCo_{1-x}O$ nanoparticles in HER and OER demonstrate great potential for the design of electrocatalysts for overall water splitting.

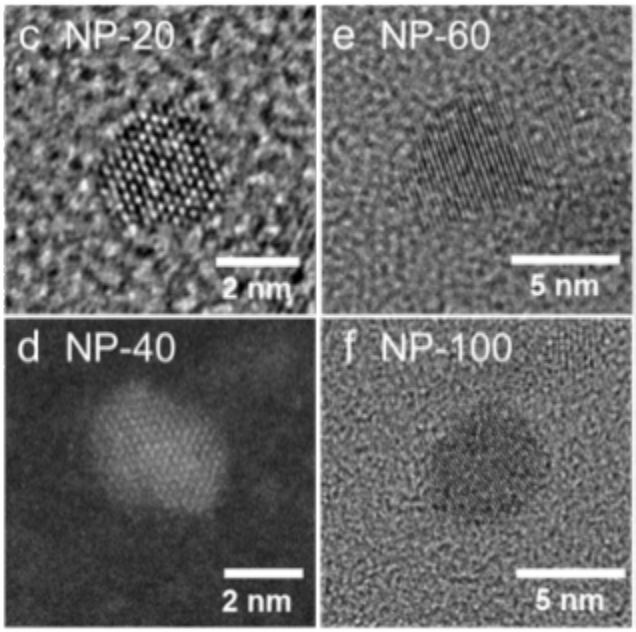


Fig. 1: High resolution transmission electron micrograph images of single $Ni_xCo_{1-x}O$ nanocrystals with c) 20 at%, e) 60 at%, and f) 100 at% Co. d) STEM image of a single nanocrystal with 40 at% Co.

- **K. Fominykh, G. C. Tok, P. Zeller, H. Hajiyani, T. Miller, M. Döblinger, R. Pentcheva, T. Bein, and D. Fattakhova-Rohlfing:** *Rock Salt Ni/Co Oxides with Unusual Nanoscale-Stabilized*

8

GENERIC TRANSPORT MECHANISMS FOR MOLECULAR TRAFFIC IN CELLULAR PROTRUSIONS

Prof. Erwin Frey (LMU Munich, Department of Physics)
■ www.theorie.physik.uni-muenchen.de/lsfrey

Cellular protrusions are finger-like extensions of a cell projecting into the surrounding environment and they play an important role in different contexts ranging from cell migration to signal transduction. Their shape is maintained by actin filaments that are cross-linked into rigid bundles. Those actin filament bundles are also essential for transport of proteins to the protrusion tips. Molecular motors help fulfil this task by converting chemical energy from ATP hydrolysis into directed movement along the filaments, pulling the proteins as cargo behind them. Furthermore, instead of being transported directionally along the filaments, the proteins can also reach the tip by diffusion in the cytosol.

In this project, we examined the interplay between active, directed transport and diffusive motion in a half-closed geometry with a conceptual, mathematical model.
Our work suggests an intriguing task-sharing mechanism: While naively, one would assume that transport of the proteins to the tip should be much faster by directed motion than by diffusion in the cytoplasm, our model predicts that directed transport is strongly suppressed, and transport to the tip is fostered by diffusion. The reduction of the active current on the filament is due to steric hindrance between the motors that cannot penetrate or overtake each other. As a result, motors accumulate at the tip, and correlations between the motors become significant.

From a biological point of view, the congestion of motors at the protrusion tip might be beneficial: It would prolong the residence time of the proteins at the tip, possibly facilitating their tasks there. We find that in order to achieve accumulation of proteins at the tip but simultaneously to avoid large traffic jams the unbinding rate of the motors at the filament tip needs to be much larger than the binding and unbinding rates in the bulk of the filament.

On a broader perspective, our study might help to understand the interplay between active and passive transport in more elaborate models, and to illustrate the role of correlations in biological systems.

■ **Isabella R. Graf, Erwin Frey:** *Generic transport mechanisms for molecular traffic in cellular protrusions*; Phys. Rev. Lett. 118 (12), 128101 (2017).

9

FORCE MEASUREMENTS ON SINGLE MOLECULES

Prof. Hermann E. Gaub (LMU München, Physics Department) ■ www.biophysik.physik.lmu.de

AFM-based Single-molecule force spectroscopy (SMFS) measures the extension of a molecule when subjected to force and allows probing its mechanical and biological properties. Protein folding can be explored by pulling on one terminus to unfold it; upon relaxation, it may refold toward its native states [1]. Such experiments revealed the importance of mechanical force as a functional regulator of biomolecules: The activity of smooth muscle myosin light chain kinase (smMLCK) was shown to depend on external forces. Its catalytic activity is triggered by a force dependent conformational change upon Ca^{2+}/calmodulin binding [2]. The mechanical stability of a cellulosomal scaffoldin was investigated in a newly developed parallelized one-pot *in vitro* transcription–translation and protein pull-down protocol by high-throughput SMFS measurements. All atom MD simulations in collaboration with the Schulten group at the Beckmann center in Urbana Illinois revealed details of its molecular mechanisms [3]. Single-molecule force spectroscopy greatly benefits from site-specific surface immobilization and specific probing with a functionalized cantilever. Covalently attaching mechanically stable receptors onto proteins of interest improves pickup efficiency and specificity. The Enzymatic sortase reaction provides such a covalent attachment for improved throughput [4]. Also elastin like polymers (ELPs) were developed to anchor molecules of interest to surfaces and/or cantilever tips since they by far perform more precise and specific compared to the common standard linker poly(ethylene-glycol) (PEG) [5]. The tetravalency of the widely used streptavidin results in diverse force propagation pathways through the different binding interfaces. This multiplicity gives rise to polydisperse force spectroscopy data. The recently engineered monovalent streptavidin tetramer with a single cysteine in its functional subunit now allows for site-specific immobilization of the molecule of interest, orthogonal to biotin binding[6]. AFM-based single-molecule cut-and-paste (SMC&P) was expanded by the recently developed Strep-Tag II [7].

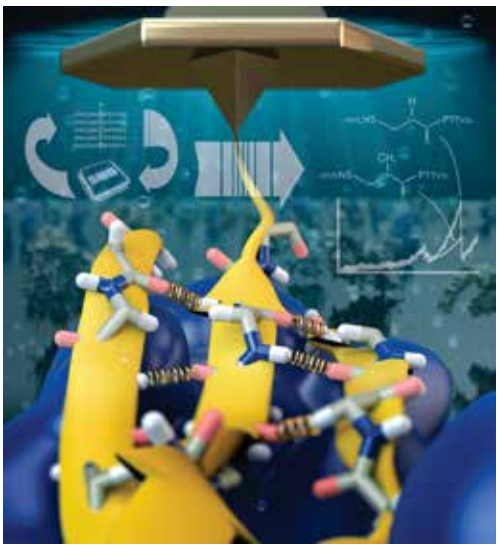


Fig. 1: The combination of steered molecular dynamics simulations (SMD) and AFM single-molecule force spectroscopy (cantilever shown in gold) allowes testing and fine-tuning the mechanical stability of cellulosomal scaffoldin protein domains (secondary structure of the molecule represented in yellow, hydrogen bonds represented by springs). One mutation, predicted by SMD, doubled the mechanostability (grey schematics) [3].

■ **[1] David Alsteens, Hermann E. Gaub, Richard Newton, Moritz Pfreundschuh, Christoph Gerber and Daniel J. Müller:** *Atomic force microscopy-based characterization and design of biointerfaces*; Nature Reviews, doi: 10.1038/natrevmats.2017.8 (2017).

[2] Fabian Baumann, Magnus S. Bauer, Martin Rees, Alexander Alexandrovich, Mathias Gautel, Diana A. Pippig, Hermann E. Gaub: *Increasing evidence of mechanical force as a functional regulator in smooth muscle myosin light chain kinase;* eLIFE, DOI: 10.7554/eLife.26473.001 (2017).

[3] Tobias Verdorfer, Rafael C. Bernardi, Aylin Meinhold, Wolfgang Ott, Zaida Luthey-Schulten, Michael A. Nash, and Hermann E. Gaub: *Combining in Vitro and in Silico Single-Molecule Force Spectroscopy to Characterize and Tune Cellulosomal Scaffoldin Mechanics;* JACS, DOI: 10.1021/jacs.7b07574 (2017).

[4] Ellis Durner, Wolfgang Ott, Michael A. Nash and Hermann E. Gaub: *Post-Translational Sortase-Mediated Attachment of High-Strength Force Spectroscopy Handles;* Omega, DOI: 10.1021/acsomega.7b00478 (2017).

[5] Wolfgang Ott, Markus A. Jobst, Magnus S. Bauer, Ellis Durner, Lukas F. Milles, Michael A. Nash, and Hermann E. Gaub: *Elastin-like Polypeptide Linkers for Single-Molecule Force Spectroscopy;* ACS Nano, DOI: 10.1021/acsnano.7b02694 (2017).

[6] Steffen M. Sedlak, Magnus S. Bauer, Carleen Kluger, Leonard C. Schendel, Lukas F. Milles, Diana A. Pippig, Hermann E. Gaub*: *Monodisperse measurement of the biotinstreptavidin interaction strength in a welldefined pulling geometry;* PLOS ONE, https://doi.org/10.1371/journal.pone.0188722 (2017).

[7] Katherine R. Erlich, Fabian Baumann, Diana A. Pippig, and Hermann E. Gaub: *Strep-Tag II and Monovalent Strep-Tactin as Novel Handles in Single-Molecule Cut-and-Past;* Small Methods, DOI: 10.1002/smtd.201700169 (2017).

[8] Daniel J. Müller and Hermann E. Gaub: *Science Perspective: Membrane proteins scrambling through a folding landscape;* Science 355 (6328), doi: 10.1126/science.aam8370 (2017).

10

MULTIPLEXING MOLECULAR TENSION SENSORS REVEALS PICONEWTON FORCE GRADIENT ACROSS TALIN-1

Prof. Carsten Grashoff (MPI of Biochemistry) ■ http://www.biochem.mpg.de/en/rg/grashoff
Prof. Matthias Rief (TU München) ■ http://bio.ph.tum.de/home/e22-prof-dr-rief/rief-home.html

Förster resonance energy transfer (FRET)-based tension sensor modules (TSMs) are available for investigating how distinct proteins bear mechanical forces in cells. Yet, forces in the single piconewton (pN) regime remain difficult to resolve, and tools for multiplexed tension sensing are lacking. Here, we report the generation and calibration of a genetically encoded, FRET-based biosensor called FL-TSM, which is characterized by a near-digital force response and increased sensitivity at 3–5 pN. In addition, we present a method allowing the simultaneous evaluation of coexpressed tension sensor constructs using two-color fluorescence lifetime microscopy. Finally, we introduce a procedure to calculate the fraction of mechanically engaged molecules within cells. Application of these techniques to new talin biosensors reveals an intramolecular tension gradient across talin-1 that is established upon integrin-mediated cell adhesion. The tension gradient is actomyosin- and vinculin-dependent and sensitive to the rigidity of the extracellular environment.

■ **P. Ringer, A. Weißl, A.L. Cost, A. Freikamp, B. Sabass, A. Mehlich, M. Tramier, M. Rief, and C. Grashoff.:** *Multiplexing molecular tension sensors reveals piconewton force gradient across talin-1;* Nature Methods 14, 1090-1096 (2017).

11

STUDYING AND OPTIMIZING CHARGE TRANSPORT IN HYBRID HALIDE PEROVSKITE SOLAR CELL MATERIALS

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Hybrid organometal halide perovskites, a class of materials revealing outstanding optoelectronic properties including large absorption coefficients and easily tunable bandgaps, have undergone a rapid development toward particularly promising candidates for integration into photovoltaic devices. Despite power conversion efficiencies currently surpassing 22% in lab scale devices, a detailed model properly explaining the extraordinary optoelectronic properties is still lacking. However, understanding the charge transport characteristics and their limiting factors in hybrid perovskites is of great importance for further optimization of photovoltaic systems derived from these materials. We examined the charge carrier mobilities in $CH_3NH_3PbI_3$ (MAPI) thin films obtained from a one-step synthesis procedure and in planar n-i-p devices based on these films using the Time-of-Flight (ToF) technique. This method is well established in the field of photovoltaic materials as it provides valuable information about the drift mobility of charge carriers, one of the key quantities determining charge transport. By performing ToF measurements, we find mobilities around 6 cm^2/Vs for electrons and holes in MAPI thin films, whereas in working solar cells the respective effective mobility values are reduced by three orders of magnitude. From complementary experiments on devices with varying thicknesses of electron and hole transport layers, respectively, we identified the charge extraction layers and the associated interfaces rather than the perovskite material itself as the major limiting factors of the charge carrier transport time in working devices.

■ **I. Grill, M. Aygüler, T. Bein, P. Docampo, N. Hartmann, M. Handloser, A. Hartschuh:** *Charge transport limitations in perovskite solar cells: The effect of charge extraction layers;* ACS Applied Materials & Interfaces 9, 37655 (2017).

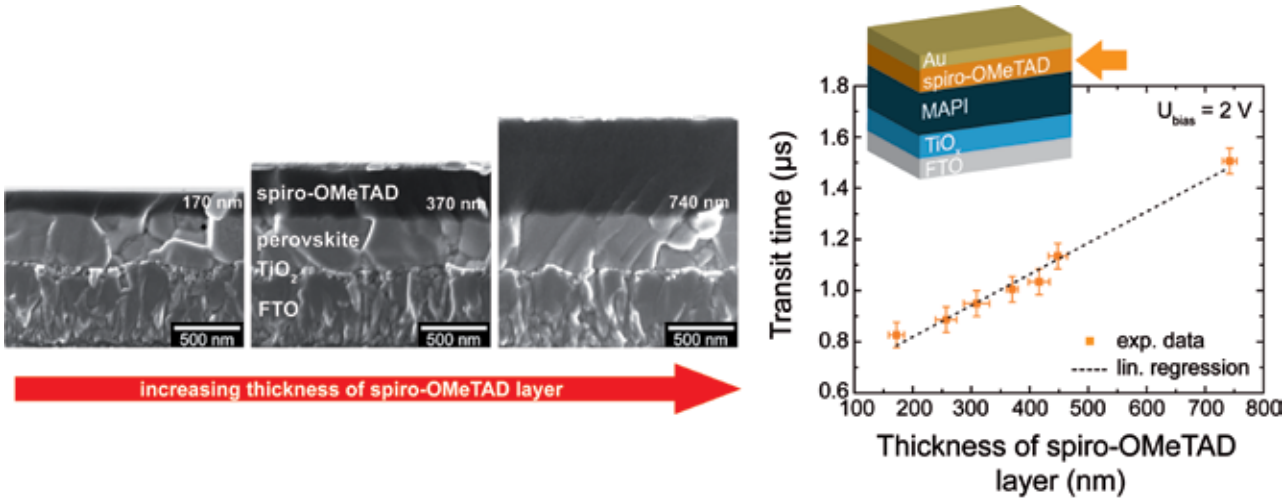

Fig 1. (Left) Cross-sectional views of the fabricated devices with increasing layer thickness of the hole transporting material spiro-OMeTAD. **(Right)** Charge carrier transport time through the whole device for increasing thickness of the hole transport layer. The charge extraction layers and the associated interfaces rather than the perovskite material itself determine the charge carrier transport time in working devices.

12

OPTO-VALLEYTRONIC IMAGING OF ATOMICALLY THIN SEMICONDUCTORS

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The past years have witnessed a new paradigm in condensed matter physics that aims at using atomically thin two-dimensional (2D) materials to build high performance electronic and optical devices. In contrast to semi-metallic graphene, atomically thin layers of transition metal dichalcogenides (TMDs) exhibit a direct band-gap and thus a sizable light-matter coupling crucial for opto-electronic applications. Moreover, circular charge currents with quantized angular momentum, described by the so-called valley index, can be generated in TMD monolayers with circularly polarized light. This feature of valley polarization is the key to the opto-valleytronic functionality with optical control over topological electron or exciton-polariton currents.
In our work, we studied the valley pseudospin optics in monolayer MoS_2, a representative TMD material. We introduced a novel method of 2D polarimetry to visualize the landscapes of valley polarization and valley coherence in extended monolayer crystals. Utilizing the sensitivity of the valley index to the crystal quality, our technique can be used to identify crystal defects such as grain boundaries or surface contaminants, thus providing direct means of opto-valleytronic inspection of layered semiconductors. Scaled from microscopic to macroscopic length scales, it will facilitate rapid and efficient inspection of wafer-scale opto-valleytronic semiconductors and heterostructures.

Fig. 1: Optical micrograph of two-dimensional crystals of the thin-film semiconductor molybdenum disulfide. Image by Hisato Yamaguchi, Los Alamos National Laboratory, USA.

■ **A. Neumann, J. Lindlau, L. Colombier, M. Nutz, S. Najmaei, J. Lou, A. D. Mohite, H. Yamaguchi, and A. Högele:** *Opto-valleytronic imaging of atomically thin semiconductors;* Nature Nanotechnology 12, 329-334 (2017).

13

COLLECTIVE EXCITATIONS IN DIPOLAR EXCITON GASES

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Long-living spatially indirect dipolar excitons in a semiconductor double quantum well are investigated, aiming for a better understanding of many-body phenomena in such dipolar exciton ensembles. Depending on confinement, excitonic densities, and temperature, the exciton interactions are expected to possibly result in phase transitions ranging from Wigner crystallization via Bose-Einstein condensation in fully confined systems to a Mott transition into an electron-hole plasma at highest densities. Nanofabricated electrostatic traps enable to confine even single to few dipolar excitons.

In a recent study, the photogenerated excitonic ensembles confined in coupled GaAs quantum wells were probed by a complementary approach of emission spectroscopy and resonant inelastic light scattering. Lateral electrostatic trap geometries were used to create dense systems of spatially indirect excitons and excess holes with similar densities in the order of 10^{11} cm^{-2}. Inelastic light scattering spectra reveal a very sharp low-lying collective mode that is identified at an energy of 0.44 meV and a full width at half maximum of only 50 μeV. This mode is interpreted as a plasmon excitation of the excess hole system coupled to the photogenerated dipolar excitons. The emission energy of the dipolar excitons shifts under the application of a perpendicular applied electric field, with the quantum-confined Stark effect unperturbed from the presence of free charge carriers. The results illustrate the potential of studying low-lying collective excitations in photogenerated exciton systems to explore the many-body phase diagrams, related phase transitions, and interaction physics.

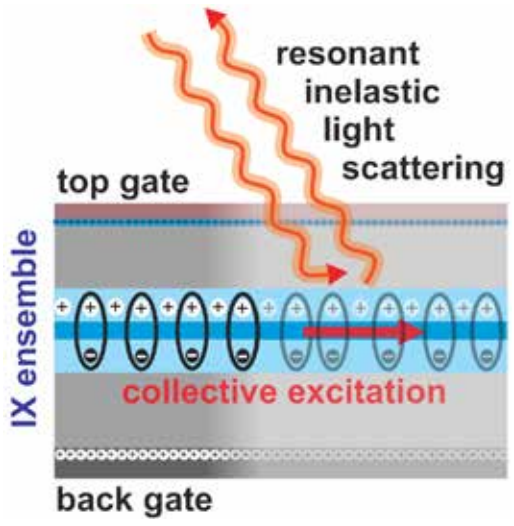

Fig. 1: Resonant inelastic light scattering allows to read-out collective excitations of dipolar exciton ensembles coherently coupled to photogenerated holes in electrostatic exciton traps with top and bottom gates.

■ **S. Dietl, S. Wang, D. Schuh, W. Wegscheider, J. P. Kotthaus, A. Pinczuk, A.W. Holleitner, U. Wurstbauer:** *Collective electronic excitation in a trapped ensemble of photogenerated dipolar excitons and free holes revealed by inelastic light scattering;* Phys. Rev. B 95, 085312 (2017).

S. Dietl, K. Kowalik-Seidl, D. Schuh, W. Wegscheider, A.W. Holleitner, U. Wurstbauer: *Overflow of a dipolar exciton trap at high magnetic fields;* Superlattices and Microstructures, special issue on indirect excitons, vol. 108, 42-50 (2017).

14

SINGLE-CHARGE SENSITIVITY IN THZ NEAR-FIELD MAPPING

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Exotic, conducting materials such as unconventional superconductors or organic conductors are of high current interest. This results from the rich physics and applications offered by correlated electrons that are entangled by charge, orbital, spin, and lattice degrees of freedom. Such correlated quantum matter is highly susceptible to external perturbation, and thus exhibits intrinsic phase complexities down to the nanometer scale. For probing the conductivity at 20 nm resolution, scattering-type optical near-field microscopy (s-SNOM) has emerged over the last two decades, but has not performed at very long infrared wavelengths which are needed for highest sensitivity. The present development demonstrates 50-nm resolved near-field imaging at = 500 µm (equiv. to 0.6 THz), enabled by a high-harmonic microwave circuit for radiating via free space to a standard s-SNOM, and at the same time detecting the back-scattered wave interferometrically. In contrast to former attempts, the system uses no laser or cryogenic detector, but houses microwave synthesizers, single-mode waveguide components, and Schottky mixers in a permanently aligned, compact transceiver that returns both amplitude and phase information to the s-SNOM's controller. The frequency can be tuned between 0.5 and 0.75 THz for determining the conductivity spectrum which reveals the density of electrons as well as their possible deviation from "free-electron" transport, induced by correlation.
Background-free amplitude and phase nano-images are recorded for the first time in the THz range. Images of Si with doped nanostructures prove a conductance sensitivity corresponding to 10^{16} cm^{-3} mobile charge carriers. With the attained spatial resolution of 50 nm, this means that the signal is due to 1.25 mobile charge carriers on average in a probing volume of 50x50x50 nm^3, i.e., that the method provides single-charge sensitivity. Analyzing an n/p transition region (Fig. 1) reveals it also distinguishes carrier type.

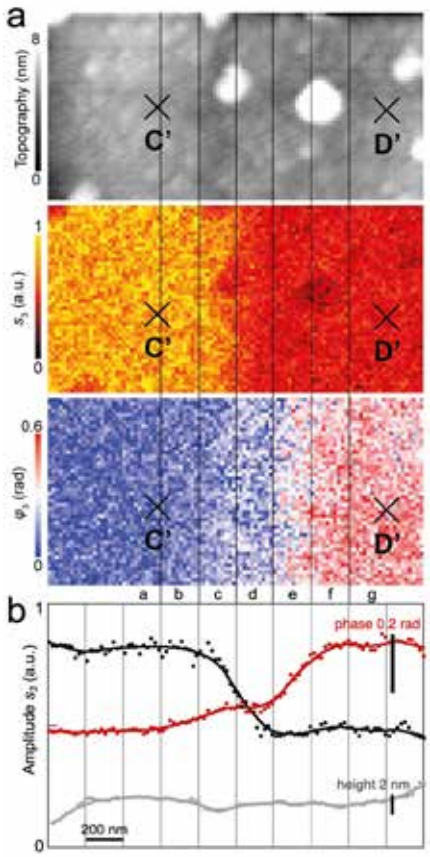

Fig. 1: s-SNOM image at 0.6 THz of n/p transition in Si; a, simultaneously recorded topography, THz amplitude s, and THz phase φ (acquisition time 2.5 min); b, line profiles of height (grey), amplitude (black), and phase (red), obtained by averaging, show that *electron* density reduces from 2 10^{17} cm^{-3} in section a along b and c to ca. 3 10^{16} cm^{-3}, while *hole* density emerges along d and e to attain a value of 2 16 cm^{-3}.

■ **C. Liewald, S. Mastel, J. Hesler, A.J. Huber, R. Hillenbrand, and F. Keilmann:** *All-electronic terahertz nanoscopy;* Optica 5, 159 (2018).

A.J. Sternbach, J. Hinton, T. Slusar, A.S. McLeod, M.K. Liu, A. Frenzel, M. Wagner, R. Iraheta, F. Keilmann, A. Leitenstorfer, M. Fogler, H.-T. Kim, R.D. Averitt, and D.N. Basov: *Artifact-free time-resolved near-field spectroscopy;* Optics Express 25, 28589 (2017).

15

SCALABLE FABRICATION OF HYBRID POLYMER/SiO_2 NANOPHOTONIC CAVITY ARRAYS WITH AN ENCAPSULATED MOS_2 MONOLAYER

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Monolayer transition metal dichalcogenides (TMDs) such as molybdenite (MoS_2) have recently attracted great interest in the field of photonics because of their distinctive optical and spin properties. In contrast to bulk TMD materials, which are indirect bandgap semiconductors, monolayer TMDs are highly optical active due to a direct bandgap ranging between 1 and 2 eV. In contrast to top-down fabrication methods like exfoliation which yields single TMD flakes of high purity, but does not permit scalability, chemical vapor deposition (CVD) generates TMD islands and continuous films of uniform layer thickness and excellent optical and electrical properties. The integration of these highly optically active materials into photonic circuits, for example as light emitters or non-linear elements, requires efficient coupling to optical fields. This can be dramatically enhanced by nanophotonic resonators.

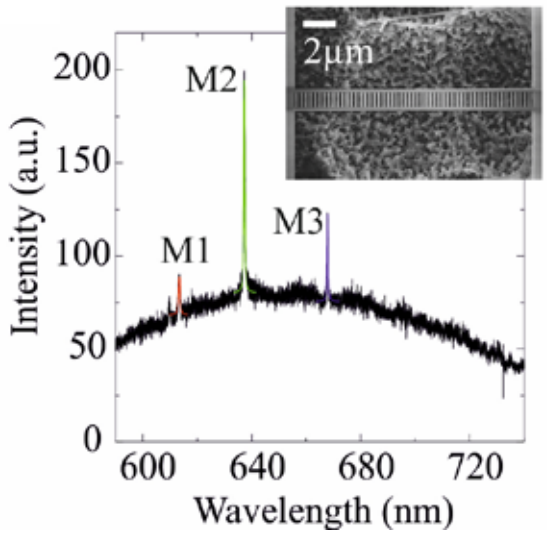

Fig. 1: Emission spectrum of a hybrid SiO_2-MoS_2-polymer photonic crystal nanocavity showing the characteristic broad MoS_2 emission decorated with three modes, M1, M2 and M3, which are fitted with Lorentzians (colored solid lines). **Inset:** electron microscope image of a fabricated device.

To this end, the fully-scalable fabrication of a large array of hybrid TMD-silicon dioxide (SiO_2) is highly desirable. We realized such fully scalable fabrication: device fabrication started by substrate-scale CVD growth of MoS_2 on non-birefringent thermal oxide on a silicon wafer; it was followed by lithographic fabrication of a photonic crystal nanocavity array on the same substrate at more than 50% yield of functional devices. The MoS_2 monolayer is fully encapsulated between the SiO_2 growth substrate and polymer electron beam resist. This encapsulation reduces degradation of the TMD and enhances its coupling to the optical mode. Our cavities exhibit three dominant modes with measured linewidths less than 0.2 nm, corresponding to quality factors exceeding 4000 (see Figure). Moreover, these modes are continuous tunability across the entire emission band of MoS_2 simply by variation of the photonic crystal periodicity.
Our fully scalable approach is ideally suited for complex large-scale nanophotonic circuits built from a toolbox of functional design elements. In such circuits the large-area CVD TMD layer will offers multiple functionalities as an optical emitter or a non-linear optical medium and a channel layer for associate drive electronics. In particular, simply by adding electrical contacts, the TMD layer can be transformed to an on-chip photodetector or a LED.

■ **S. Hammer, H. M. Mangold, A. E. Nguyen, D. Martinez-Ta, S. Naghibi Alvillar, L. Bartels, H. J. Krenner:** *Scalable Transfer-Free Fabrication of MoS_2/SiO_2 Hybrid Nanophotonic Cavity Arrays with Quality Factors Exceeding 4000;* Scientific Reports 7, 7251 (2017).

16

POST-SYNTHETIC DECOUPLING OF IN-SITU SYNTHESIZED ORGANIC NANOSTRUCTURES FROM METAL SURFACES

PD Dr. Markus Lackinger, Prof. Wolfgang M. Heckl (TU München, Department of Physics and TUM School of Education, and Deutsches Museum)

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Novel extended covalent organic nanostructures can be synthesized by direct polymerization of functional monomers on solid-surfaces. In most cases of this so called on-surface synthesis, chemical contributions of reactive metal surfaces are required to drive the reaction. Consequently, the organic nanostructures become adsorbed on these strongly interacting supports, whereby their structural and electronic properties can become considerable altered. Hence, means for alleviating the substrate influence by decoupling are highly desirable. Therefore, the Lackinger group proposed and studied intercalation of iodine monolayers between the covalent networks and the metal supports as an effective method for post-synthetic decoupling. They have shown that this can readily be accomplished by exposing the as synthesized, i.e. metal-supported, covalent networks to iodine vapor. While on silver surfaces exposure at room temperature is already sufficient, they could demonstrate that a protocol with elevated sample temperatures is required for the implementation on technologically more relevant gold surfaces. Iodine intercalation is detectable in various microscopic and spectroscopic signatures, for instance as characteristic changes in photoemission or X-ray absorption spectra. Most evidently, the Scanning Tunneling Microscopy contrast changes markedly from a featureless appearance of the directly on-metal adsorbed networks to a "cloudy" appearance after successful decoupling. The latter corresponds to the frontier molecular orbitals of free-standing networks, and can hence be interpreted as efficient electronic decoupling from the metal supports.

Post synthetic decoupling of on-surface synthesized covalent nanostructures by intercalation of iodine monolayers not only facilitates the characterization of the networks intrinsic properties, but might also promote first applications that crucially rely on their unperturbed electronic structure.

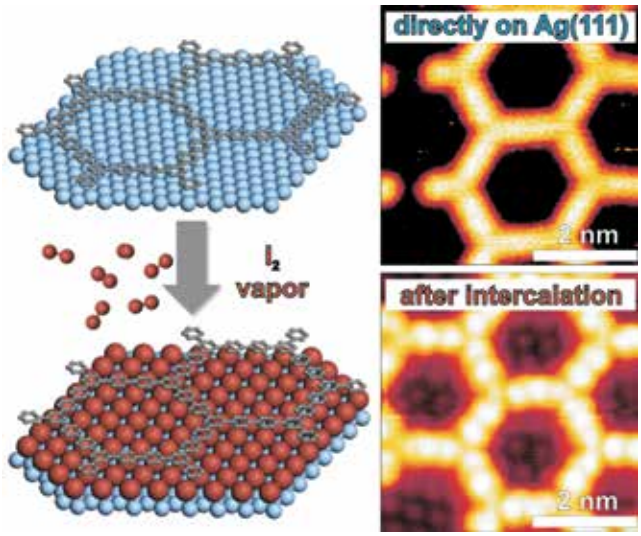

Fig. 1 (Left): scheme of post-synthetic decoupling by intercalation of an iodine monolayer; **(Right)** STM images comparing the mostly featureless contrast before with the "cloudy" contrast after decoupling of a covalent hexagonal network with triazine and biphenyl moieties at its corners and edges, respectively.

■ **A. Rastgoo-Lahrood, M. Lischka, J. Eichhorn, D. Samanta, M. Schmittel, W.M. Heckl, M. Lackinger:** *Reversible Intercalation of Iodine Monolayers between on-Surface Synthesised Covalent Polyphenylene Networks and Au(111);* Nanoscale 9, 4995 (2017).

17

ASSEMBLY OF ROTAVIRUS

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Rotaviruses are highly-infectious RNA-containing viruses that infect children. Currently, there is no available treatment after a child is infected. The rotavirus contains 11 RNA segments, of which a single copy of each segment is efficiently packed into a forming virus. How the viruses manage to count up to 11 is not known although certainly RNA-RNA and protein-RNA interactions are important.

To investigate this early step in the assembly of rotavirus, Borodavka et al used fluorescence cross-correlation spectroscopy (FCCS) and systematic evolution of ligands by exponential enrichment (SELEX). Using fluorescently labeled segments of rotavirus RNA, Borodavka et al used FCCS to show minimal RNA-RNA interactions. However, in the presence of the non-structural viral protein, NSP2, a significant increase in cross-correlation was observed, indicating RNA-RNA interactions (Fig. 1A). To investigate the structural changes induced by NSP2 in detail, SELEX experiments were performed on segment 11 in the absence and presence of NSP2 (Fig. 1B). Using SELEX, we could identify regions of single-stranded RNA within segment 11 and look for possible complimentary sequences in the other 10 segments. Upon addition of NSP2, significant structural rearrangements of the RNA segments could be observed, which enable RNA-RNA interactions with the other segments.

To test the results of the SELEX experiments, we made mutations to the region of segment 5 or segment 11 that we found should interact. Mutations in this region to either segment 5 or 11 significantly reduced the interactions between segments as visualized with FCCS. These experiments suggest a role of NSP2 in rearranging the RNA for packaging (Fig. 1C) and open the door for investigating RNA-RNA interactions in the absence and presence of proteins. By elucidating the pathway of viral assembly, an understanding of the RNA-RNA interaction network becomes possible, which will expedite the development of potential vaccines.

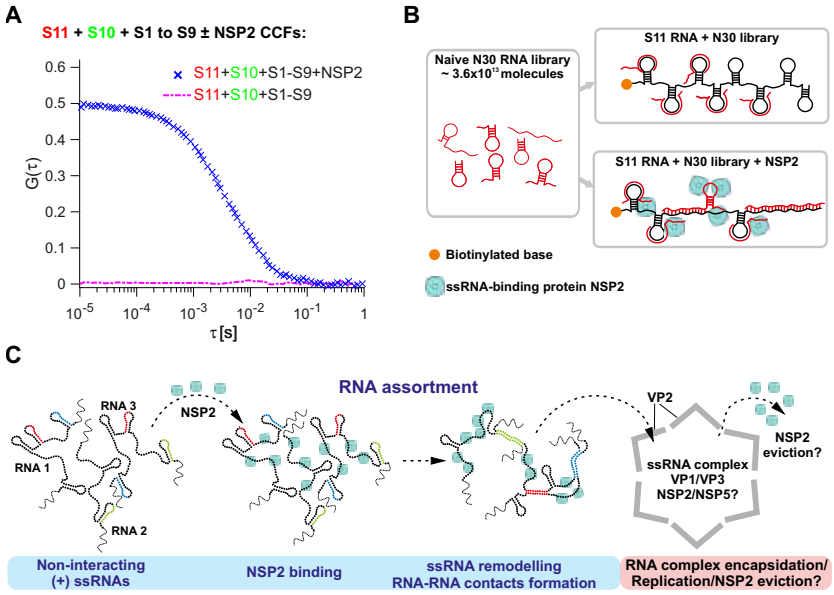

Fig. 1: The Role of NSP2 in Rotavirus Assembly. **A)** FCCS measurements with fluorescently labeled segments S10 and S11 (in the presence of unlabeled segments S1 and S9) from rotavirus showing a significant increase in cross-correlation signal upon addition of the non-structural protein, NSP2. **B)** A schematic of SELEX measurements showing the binding of 30 bp RNAs to single-stranded regions of segment S11 in the absence and presence of NSP2. Thereby, we can detect NSP2 induced structural rearrangements of the segment 11 RNA. **C)** A model of rotavirus RNA assembly where binding of NSP2 rearranges the viral RNA such that it can package a single copy of each RNA.

■ **A. Borodavka, E.C. Dykeman, W. Schrimpf, and D.C. Lamb:** *Protein-mediated RNA folding governs sequence-specific interactions between rotavirus genome segments;* eLife 6, e27453 (2017).

18

HOTSPOT-MEDIATED NON-DISSIPATIVE AND ULTRAFAST PLASMON PASSAGE

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Most of the energy consumed by today's computers is converted into useless heat as classical processors perform their calculations by moving around charges on semiconductor transistors. As an alternative, photons are explored as processing entities but also as mediators of the generated information. Ideal future devices for all-optical-based computing could thus simply transfer light between computing subunits eliminating the charge-related production of heat. Essential requirements for photon conducting elements would be high transfer efficiency, low energy losses and fast transfer times. Linear arrangements of metallic nanoparticles of identical material, usually gold, have long been proposed to serve as such photonic wires. However, these suffer from large energy losses as the photons "ride" on plasmons, which are again oscillations of charges in the particle chains. To avoid the resulting electron-induced heat losses, we here propose theoretically and prove experimentally a new concept for efficient and fast photon transfer: instead of using only gold particles, we introduce a silver particle that acts as transmitter between two communicating gold particles. Importantly, the plasmon in the silver particle is here in an inaccessible state of energy for the gold plasmon and hence participates only virtually in the transfer process. As a result, no heat is generated in the silver particle while the two gold particles are still perfectly coupled. For the experimental realization of our transfer system we needed full control over the spatial organization of nanoparticles of two materials, which is impossible to achieve with standard fabrication methods. Using DNA nanotechnology, we were able to build self-assembling chains of 40 nm gold and silver particles consisting out of three metal nanoparticles. We demonstrated loss-less coupling between the two remote gold nanoparticles and showed plasmon transfer on the femtosecond scale. With that, an ultra-fast non-dissipative passage of plasmons was realized opening the door towards a new class of plasmonic wave-guides.

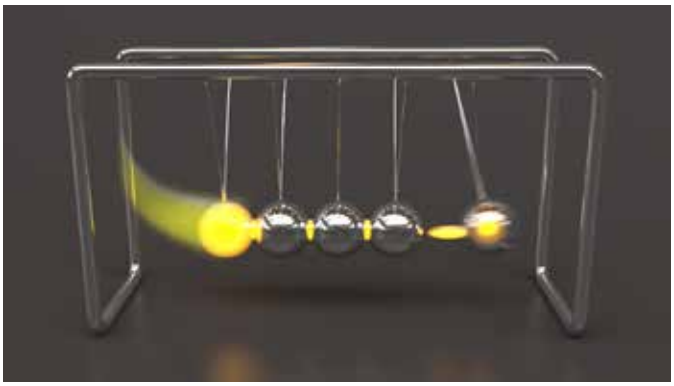

Fig. 1: „A Newton cradle visualizes the idea of moving energy from one end of a particle chain to the other, and then back and forth again. Just as we see it happening with the plasmon wave package oscillating between the different ends in a hetero-nanoparticle chain." Illustration: Christoph Hohmann, NIM.

■ **E.-M. Roller, L. V. Besteiro, C. Pupp, L. Khosravi Khorashad, A. O. Govorov, T. Liedl:** *Hotspot-mediated non-dissipative and ultrafast plasmon passage;* Nature Physics 13, 761–765 (2017).

19

DIRECTIONAL PHOTONIC WIRE MEDIATED BY HOMO-FÖRSTER RESONANCE ENERGY TRANSFER ON A DNA ORIGAMI PLATFORM

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Prof. Don C. Lamb (LMU München, Department of Chemistry)
■ www.cup.uni-muenchen.de/pc/lamb

The homo-FRET phenomenon (fluorescence energy transfer among fluorophores of the same kind) is exploited in biology by the light harvesting complex and in nanotechnology for the construction of photonic wires. Despite its many applications, there are very few studies focused on addressing the complexity of the phenomenon per se. In this work, DNA origami was used to build homo-FRET nano-wires. Through the combination of bulk experiments, single molecule spectroscopy and theoretical modeling, new insights on the role of homo-FRET in assemblies of florophores has been gained. By exploiting the spatial programmability of DNA origami to arrange fluorophores in a variety of configurations with nanometer precision, the precise evaluation of the contribution of each homo-FRET dye, specifically Cyanine 3, to the energy migration depending on their relative position was possible. As a proof of concept, the homo-FRET system was used to build a photonic nano-wire, which can efficiently transfer energy over a distance of 16 nm, which is approximately twice the distance possible for a common hetereo-FRET pair.

■ **F. Nicoli, A. Barth, W Bae, F. Neukirchinger, A. H. Crevenna, D. C. Lamb, T. Liedl:** *Directional Photonic Wire Mediated by Homo-Förster Resonance Energy Transfer on a DNA Origami Platform;* ACS Nano 11, 11264–11272 (2017).

20

MOLECULAR FORCE SPECTROSCOPY WITH A DNA ORIGAMI-BASED NANOSCOPIC FORCE CLAMP

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Here we describe how we constructed self-assembling, nanoscopic force clamps to study biomolecules under constant, adjustable forces in the low picomolar range. This molecular force clamps constitute a completely new concept that will complement current force spectroscopy assays. They feature several distinct properties that allowed us and will allow others to perform such measurements in previously inaccessible molecular systems and in unprecedented quality at low forces. (i) The self-assembled devices act fully autonomously as no physical connections to the outside world, such as long tethers and surfaces, are required. (ii) Simple optical reporting allows accurate detection of molecular fluctuations at millisecond resolution and under adjustable forces. (iii) Instead of creating forces "artificially" through optical or magnetic traps or by pulling with AFM cantilevers, the forces in our system are generated through the statistical fluctuations / entropic spring behavior of a biomolecule that is nanoscopic itself. When considering that molecular forces are generally the result of statistical fluctuations, you may agree that ours is the most natural way of generating forces. (iv) The nanoscopic size of our DNA-based force clamps and their inherent biocompatibility enables precise and programmable interaction with a wide range of molecular systems. (v) The easy manufacturing of DNA origami structures that self-assemble at high yields results in massive parallelization of measurements and high data throughput. (vi) Our approach can be combined with all other features of DNA nanotechnology, including super-resolution imaging and biological targeting.

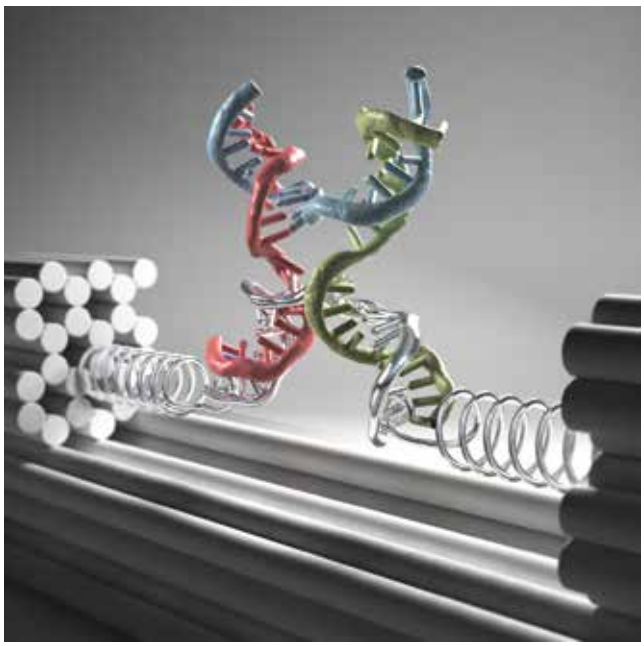

Fig. 1: Nanoclamp made of DNA strands. Illustration: Christoph Hohmann, NIM.

■ **P. C. Nickels, B. Wünsch, P. Holzmeister, W. Bae, L. M. Kneer, D. Grohmann, P. Tinnefeld, T. Liedl:** *Molecular force spectroscopy with a DNA origami–based nanoscopic force clamp;* Science 354, 6310, pp. 305-307 (2016).

21

COATINGS OF PURIFIED GASTRIC MUCINS PREVENT TISSUE DAMAGE IN OCULAR TRIBOLOGY

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■ www.imetum.tum.de/forschung/biologische-hydrogele

With a prevalence of more than 10%, keratoconjunctivitis sicca (commonly known as dry eye syndrome) is one of the most frequent forms of ocular diseases; among contact lens wearers, this condition occurs even more often. Key components of the protective tear film are mucins, large glycoproteins that serve as molecular lubricants on many epithelial body surfaces. It is likely that, in the absence of a proper mucinous lubrication layer on the cornea surface, increased friction and tissue damage induced by contact lens sliding lead to discomfort. Herein, it is shown that purified gastric mucins efficiently prevent damage on the cornea, when they are used as a solution for cornea lubrication or as a molecular layer for contact lens coating. Furthermore, these results suggest that such a mucin coating also improves the performance of state-of-the-art hydrogel lenses, which are designed to provide an auto-lubrication mechanism upon contact with the eye. Thus, eye drops or contact lens storage solutions containing purified gastric mucins could be a great tool in fighting ocular dryness.

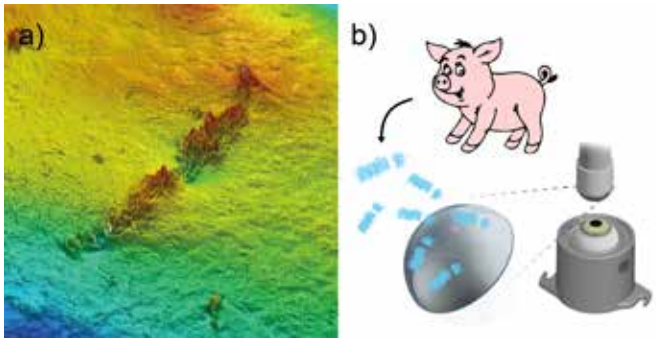

Fig. 1: (a) Three-dimensional topographical image of a local tissue damage (stripe in the middle of the image) on a cornea sample after a friction experiment conducted with an uncoated contact lens. **(b)** Purified mucins (light-blue) from pig stomachs form a protective layer on contact lenses. The tribological experiments were performed with porcine eyes (down right). (Images: B. Winkeljann / TUM)

■ **B. Winkeljann, K. Boettcher, B. Balzer and O. Lieleg:** *Mucin coatings prevent tissue damage at the cornea-contact lens-interface;* Advanced Materials Interfaces, (4) 19, 1700186 (2017).

22

CHARACTERIZATION OF FIBRIL STRUCTURAL INHOMOGENEITY OF TAU PAIRED HELICAL FILAMENTS ON THE MOLECULAR LEVEL

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As a major microtubule-binding protein, Tau plays an important role for cellular architecture and cell division. Tau paired helical filaments are fibrils that are erroneously generated from Tau in the course of Tauopathies like Parkinson's disease due to its amyloidogenic properties. Their role in the disease progress is to-date incompletely understood, and which properties of Tau and other amyloidogenic properties lead to aggregation and finally fibril formation has remained a pressing question for a broad range of neurodegenerative diseases.

Tau fibrils can be obtained *in vitro* with similar properties as in the pathological context in the presence of negatively charged interaction partners. They display a large degree of disorder (polymorphism) both on the atomic as well as on the macroscopic (i.e., micrometer) level. Using solid-state NMR spectroscopy on the Tau construct K19, Linser and coworkers were able to show that despite the overall disorder in a particular region of the Tau primary structure, the so-called hexapeptide region, the molecular constitution is reproduced both regarding the individual fibrils within a single sample as well as upon variations of fibrillization conditions. Interestingly, the same stretch that displays this structural reproducibility has been identified earlier as the region in which monomeric Tau in solution interacts with surface-bound Tau monomers. As such, the intermolecular interactions in solution translate into structurally well-defined fibril elements after aggregation, whereas the weakly interacting stretches are localized to less defined parts of the eventual fibril. This observation identifies the hexapeptide region as the constitutive sequence element for the energetic incentive of amyloidogenesis in Tau.

It remains to be seen if similar relationships between monomer interactions and eventual fibril constitution are valid for other amyloidogenic proteins and how this feature can be exploited pharmacologically to prevent the aggregation in the disease.

■ **S. Xiang, N. Kulminskaya, B. Habenstein, J. Biernat, K. Tepper, M. Paulat, C. Griesinger, S. Becker, A. Lange, E. Mandelkow, R. Linser:** *A two-component adhesive: Tau fibrils arise from a combination of a well-defined motif and conformationally flexible interactions*; J. Am. Chem. Soc., 139, 2639–2646 (2017).

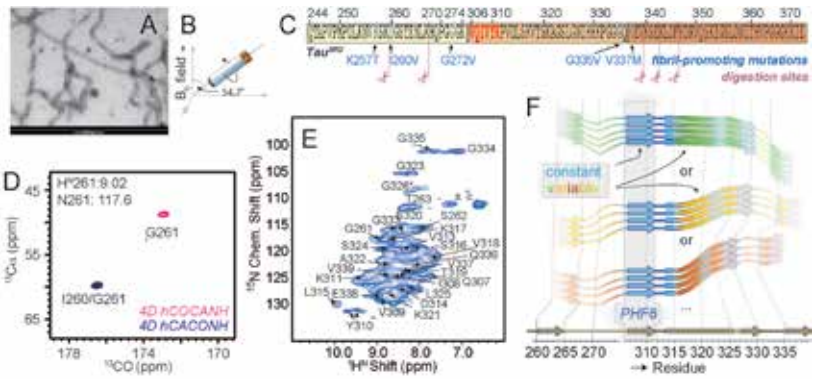

Fig. 1: The hexapeptide region constitutes not only the stretch with which monomeric Tau molecules interact, but also represents the part of the fibril that displays highest order. **A)** Tau PHF electron micrograph, **B)** representation of a Magic-Angle Spinning solid-state NMR rotor, **C)** Tau K19 primary structure with known disease mutions (blue), cleavage sites (purple) and the hexapeptide motif (red), **D)** representation of 4-dimensional solid-state NMR assignment experiments dedicated for inhomogeneous samples (Xiang et al. Chem. Commun 52, 4002-4005 (2016)), **E)** assigned 2D H/N correlation of Tau PHFs, **F)** representation of the homogeneous hexapeptide motif within the inhomogeneous fibril architecture.

23

STRETCHING AND HEATING SINGLE DNA MOLECULES WITH OPTICALLY TRAPPED GOLD-SILICA JANUS PARTICLES

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A team of researchers from the labs of Jochen Feldmann and Jan Lipfert has developed a new approach to manipulating single-molecules by applying both forces and local temperature gradients. The method is based on so-called Janus particles. Named after the two-faced Roman god Janus, these micro-meter sized particles have two distinct sides or "faces": On one side they are regular silica particles as are routinely used in optical traps; however, their other face is coated with a thin layer of gold that give them unique properties. The Feldmann lab has previously shown that if the Janus particles are placed in an optical trap, i.e. in the focus of an intense laser beam, they do not simply sit in the focus as regular optically trapped particles do, but are axially displaced from the focus due to a balance of optical and self-thermophoretic forces, since the gold face of the particles is efficiently heated by the laser (Nedev, et al., ACS Photonics, 2015; Simoncelli, et al., Small, 2016). Therefore, the height of the particle above the flow cell surface can be controlled by simple changing the laser power without altering its focus position. In this work, the particles were tethered to a flow cell surface using functionalized double-stranded DNA molecules. The DNA molecules could be efficiently stretched using the Janus particle "microscale elevator"; at the same time, the local heating close to the gold face of the Janus particle was sufficient to melt the two strands of the DNA, such that the observed stretching response is intermediate to what is expected for double- and single-stranded DNA. In the future, the ability to stretch and local heat biological macromolecules demonstrated in this proof-of-concept work will be further refined as it provides a powerful new approach in the single-molecule toolkit.

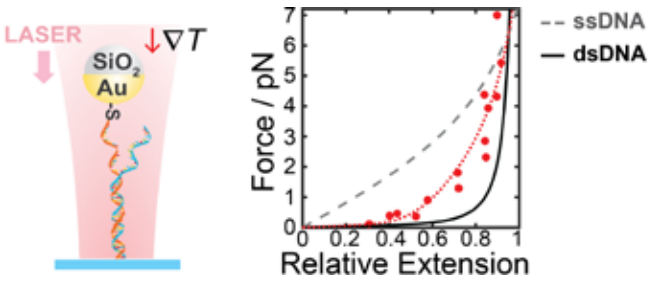

Fig. 1 (Left): Schematic of a Janus particle in an optical trap and tethered to a surface via a DNA molecule. The gold face of the particle is heated by the trapping laser; as a consequence, the DNA locally melts and the equilibrium position of the particle is above the focus of the trapping laser due to thermophoretic forces. **(Right)** Measured stretching response of a DNA molecule (red circles) manipulated by the Janus particle. The observed stretching response lies between the behaviors of a completely double- or single-stranded molecules (dashed and solid lines), indicative of partial melting.

■ **Sabrina Simoncelli*, Samuel Johnson, Franziska Kriegel, Jan Lipfert*, and Jochen Feldmann:** *Stretching and heating single DNA molecules with optically trapped gold-silica Janus particles;* ACS Photonics, 4:2843–2851 (2017). (*Joint corresponding authorship)

24

TOWARD AN AQUEOUS SOLAR BATTERY: DIRECT ELECTROCHEMICAL STORAGE OF SOLAR ENERGY IN CARBON NITRIDES

Prof. Bettina V. Lotsch (LMU Munich, Department of Chemistry and MPI for Solid State Research, Stuttgart) ■ www.cup.uni-muenchen.de/ac/lotsch

As today's society is facing a shortage of fossil fuels going in hand with climate change, new solutions for both practical and affordable energy storage devices from abundant sources are in high demand. To overcome the discrepancy between energy consumption and access to the fluctuating energy produced by renewables sources, the conversion of sunlight into solar fuels by means of photocatalysis, or into electrical energy which can be stored in batteries, are two viable solutions. In this work, the group of Bettina Lotsch has shown that cyanamide functionalized poly(heptazine imide), NCN-PHI, can be used as a photoanode in a solar battery device acting as both photoabsorber and electrical storage material at the same time. This dual functionality is unprecedented and significantly reduces the complexity of existing solar battery concepts, which invariably are dual architectures composed of a separate absorber and charge storage system.

NCN-PHI is a 2D polymer consisting of imide bridged heptazine units. The material's ability to stabilize and, thus, "store" photo-generated electrons in its backbone has previously been used to decouple hydrogen production from solar irradiation with a time delay of several hours (Lotsch et al, Angew. Chem. Int. Ed. 2017, 56, 510). This storage ability has now been exploited to develop a conceptually new solar battery photoanode based on a single material - NCN-PHI - working with a purely aqueous electrolyte. While the NCN-PHI backbone is (photo)reduced, the negative charge is stabilized by the adsorption of electrolyte cations within the polymer pores and at the polymer – electrolyte interface. Since the overpotential for hydrogen evolution on NCN-PHI is high, the described pseudocapacitive behavior occurs below the water reduction potential, thus enabling higher cell voltages and energy densities for aqueous batteries. The amount of solar energy that can be stored

Fig. 1: Illustration of the tandem solar cell – battery functionality, enabled by the ability of the 2D carbon nitride NCN-PHI to both absorb sunlight and to store photogenerated electrons in the form of ultra long-lived radicals. Illustration: Christoph Hohmann, NIM.

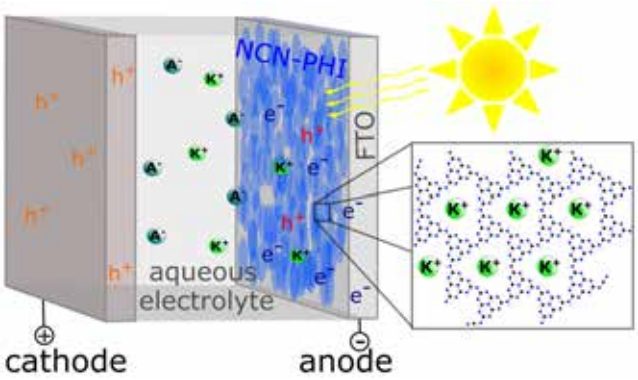

Fig. 2: Schematic of the two-electrode "solar battery" concept based on the dual photoabsorber / electron storage functionality of NCN-PHI. The inset shows the molecular structure of NCN-PHI, which hosts potassium ions in its pores that screen the photogenerated electrons.

within the material increases with illumination duration and the potential remains stable over hours, allowing for significantly delayed discharge times.

■ **F. Podjaski, J. Kröger, B. V. Lotsch:** *Toward an Aqueous Solar Battery: Direct Electrochemical Storage of Solar Energy in Carbon Nitrides;* Adv. Mater., accepted, DOI: 10.1002/adma.201705477 (2018).

V.W.-h. Lau, D. Klose, H. Kasap, F. Podjaski, M.-C. Pignié, E. Reisner, G. Jeschke, B.V. Lotsch: *Dark photocatalysis: Storage of solar energy in carbon nitride for time-delayed hydrogen generation;* Angew. Chem. Int., DOI: 10.1002/anie.201608553 (2017).

V.W.-h. Lau, V.W.-z. Yu, F. Ehrat, T. Botari, I. Moudrakovski, T. Simon, V. Duppel, E. Medina, J. Stolarczyk, J. Feldmann, V. Blum, B.V. Lotsch: *Urea-modified carbon nitrides: Enhancing photocatalytic hydrogen evolution by rational defect engineering;* Adv. Energy Mater., DOI: 10.1002/aenm.201602251 (2017).

25

PROTON GRADIENTS AND PH OSCILLATIONS EMERGE FROM HEAT FLOW AT THE MICROSCALE

Dr. Christof Mast (LMU München, Physics Department) ■ www.biosystems.physik.lmu.de

The group around Christof Mast could improve techniques to produce highly controlled thermal gradients that allow high throughput thermophoretic accumulation measurements: A specially engineered motorized microscope sequentially scans up to 12 reaction vessels, which significantly shortens the measurement times for the time-consuming "thermal trap" experiments. With this method, the group was able to extend measurements of escalated polymerization, which show sequential and enantioselective effects, with a non-equilibrium driven formation of DNA hydrogel. This effect could play a key role in breaking spontaneous sequence and chiral symmetry during the formation of life.

The current implementation of thermal reaction chambers consists of a light-curing resin that defines the microfluidic structure, which is coated on a cooled silicon wafer and covered with a heated transparent sapphire window. This method makes it possible to expand and modify reaction volume and geometry almost at will and facilitates the construction of a thermally driven "pH accumulator". Under normal circumstances, pH gradients are difficult to build up and maintain due to the high mobility of hydrogen nuclei. Living systems use phosopholipid membranes and proton pumps that require chemical energy to produce pH gradients, while prebiotic conditions cannot provide such a sophisticated machinery. The Christof Mast group was able to show that the charge-dependent thermal accumulation of buffer ions, but also simple amino acids, can locally shift the pH value and produce pH differences of up to two units via the reaction vessel. This could have been an ideal starting point for proto-cells to change thermally between the different zones of the external pH value and to use the pH differences generated via the membrane to synthesize high-energy compounds.

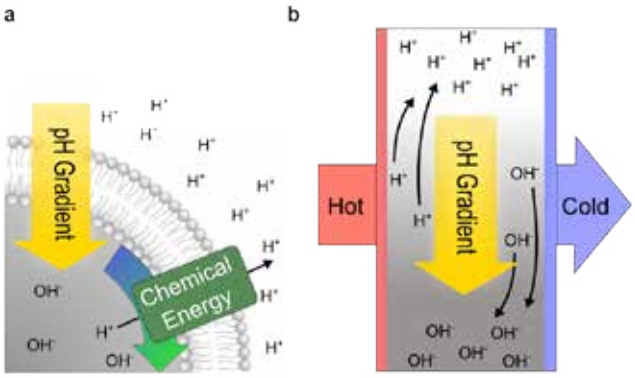

Fig. 1: Formation of pH gradients by chemical or thermal energy. **A)** Modern cells run on an elaborate protein system to maintain proton gradients across a membrane. Chemical energy is used to pump protons against their concentration gradient which is then harnessed by chemiosmosis. **B)** Heat fluxes across confined solutions, a common geological setting, induce a movement of ions that results in a stable pH gradient of up to 2 pH units. The charge selective thermophoretic accumulation of buffer molecules such as amino acids, phosphates, or nucleotides keeps the water self-ionization persistently out of equilibrium. The formation of a pH gradient is achieved in a closed system and biomolecules are repetitively exposed to differences in pH.

■ **L. Keil, F. Möller, M. Kieß, P. Kudella and C. B. Mast:** *Proton Gradient and pH oscillations emerge from heat flow at the microscale;* Nature Communication 8, 1897, doi:10.1038/s41467-017-02065-3 (2017).

26

COLOUR TUNING IN METAL-HALIDE PEROVSKITES: A MICROFOCUS & HIGH ENERGY X-RAY STUDY OF NANOCRYSTALS IN NANOPORES

PD Dr. Bert Nickel (LMU München, Physics Department)

■ www.softmatter.physik.uni-muenchen.de/nickel_group

Metal-halide perovskites are inexpensive and easily processable next generation semiconductors. For metal-halide perovskites, previous colour tuning approaches vary between altering halide stoichiometry and synthesis of colloidal particles [1]. Here, a perovskite solid-state confinement in nanoporous oxide matrices was demonstrated as a general strategy to control size of the nanocrystallites (< 10 nm) in the region were strong quantum size effects occur [2].

Preparation of nanoporous Si and Alumina films is a galvanostatic electrochemical procedure which yields a network of pores. Current density affects the pore diameter. By reducing the current density and hence the pore size, normally infrared-emitting perovskites become visibly red, and green-emitting materials become cyan or blue [2]. Wide angle X-ray scattering (WAXS) was used to investigate the size of the crystallites that form within the porous layers. The microfocussed high energy (~100 keV) X-ray beam at P07 at PETRA III allowed us to probe the perovskite filled porous layers with the incident beam parallel to the sample surface [2,3]. The resulting diffraction patterns (Fig.1a) show broadened Debye rings resulting from the perovskite crystallites. Fig.1b

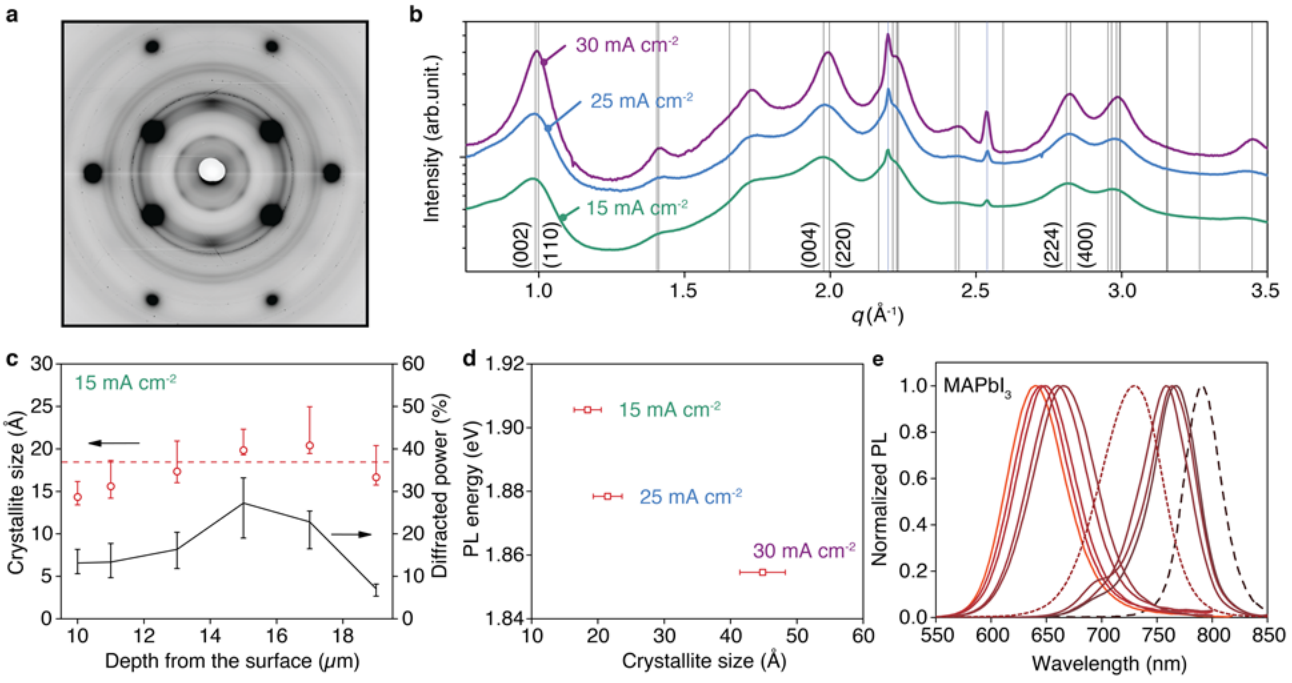

Fig. 1 a) Diffraction pattern of $MAPbI_3$ nanocrystallites in a nanoporous Si film. The image is a superposition of the scattering from the nanoporous Si and continuous broad Debye rings from the perovskite crystallites within the pores. **b)** Background corrected, azimuthally averaged intensity profiles of $MAPbI_3$ nanocrystals in nanoporous Si etched at different current. **c)** Crystallite size as function of depth for $MAPbI_3$ confined in nanoporous Si etched at 15 mA cm^{-2}. Red circles: Depth-dependent crystallite size. Dashed red line: Weighted average of the crystallite size. **d)** PL peak emission energy against the average size of crystallites formed in three nanoporous Si layers prepared with indicated anodization current density. **e)** PL spectra of $MAPbBr_3$ confined in different nonporous Si (lines) Alumina film (dots)and the bulk reference for $MAPbBr_3$ (dash).

shows diffraction profiles for three porous layers filled with $MAPbI_3$. Analogous diffraction profiles were acquired at different depths within the porous layers and the depth-dependent sizes of the $MAPbI_3$ crystallites were calculated for different samples using the Scherrer equation. In Fig.1c the sizes for $MAPbI_3$ in a porous Si layer that was etched at 15 mA cm^{-2} are presented. The decrease of the average crystallite size with decreasing current density translates directly into an increase of the PL peak emission energy (Fig.1d). This strongly indicates that the observed blue shifts can be attributed to quantum size effects. Other pore and crystallite sizes can be achieved by adjusting the current density allowing to control the peak PL wavelength (Fig.1e). From additional SAXS measurements performed at P08 at PETRA III, we estimate an average pore diameter of 4.0 nm in nanoporous Si. This is bigger than the average crystallite size within these pores (4.0 nm vs 1.8 nm).
In short, we introduced a promising method to tune the optical properties of metal halide perovskites by confining their growth in nanoporous thin films.

■ **[1] L. Polavarapu, B. Nickel, J. Feldmann, A. S. Urban:** *Advances in quantum-confined perovskite nanocrystals for optoelectronics (mini-review);* Advanced Energy Materials (2017).

[2] S. Demchyshyn, J.Roemer, H. Groiss, H. Heilbrunner, C. Ulbricht, D. Apaydin, A. Böhm, U. Ruett, F. Bertram, G. Hesser, M. Scharber, N.S. Sariciftci, B. Nickel, S. Bauer,. E.D. Głowacki, M., Kaltenbrunner: *Confining Metal-Halide Perovskites in Nanoporous Thin Films*; Science Advances (2017).

[3] Stepan Demchyshyn, Janina M. Roemer, Heiko Groiß, Herwig Heilbrunner, Christoph Ulbricht, Dogukan Apaydin, Anton Böhm, Uta Rütt, Florian Bertram, Günter Hesser, Markus Clark Scharber, Niyazi Serdar Sariciftci, Bert Nickel, Siegfried Bauer, Eric Daniel Głowacki and Martin Kaltenbrunner: *Colour tuning in metal-halide perovskites through confinement in nanoporous thin films;* DESY PHOTON SCIENCE, Highlights and Annual Report (2017).

27

EFFICIENT AND ACCURATE AB INITIO BORN-OPPENHEIMER MOLECULAR DYNAMICS FOR LARGE MOLECULAR SYSTEMS

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■ www.cup.lmu.de/pc/ochsenfeld/

The simulation of dynamic effects of molecular systems is often crucial for providing direct links between theory and experiment, e.g., for sampling potential energy surfaces, predicting experimental spectra, or calculating thermodynamic properties. Typically, observables are obtained as means or integrals of properties requiring many time steps for sufficient sampling to yield accurate results. However, so far simulations for large molecular systems at the quantum-chemical (ab initio) level were extremely costly or even impossible.
In our present work, we have combined our fast methods for performing quantum-chemical calculations on graphics processing units (GPUs) with recent developments from the fields of BOMD (extended Lagrangian BOMD) and electronic structure theory (corrected small basis set Hartree-Fock, HF-3c) for an efficient description of dynamic effects. The resulting method enables accurate simulations of large molecular systems with more than 100 atoms and explicit solvent molecules at a reasonable time scale.
To demonstrate one possible application, infrared (IR) spectra of β-carotene (Figure 1) and liquid water (Figure 2) have been determined from dipole moments sampled along BOMD trajectories. The simulated spectra are in good agreement with experimental ones. Positions, relative intensities, and shapes of the peaks are described remarkably well. Even the challenging features of the liquid water IR spectrum (e.g., the liquid water band) can be reproduced, when the number of water molecules is sufficiently large (about 100 water molecules).

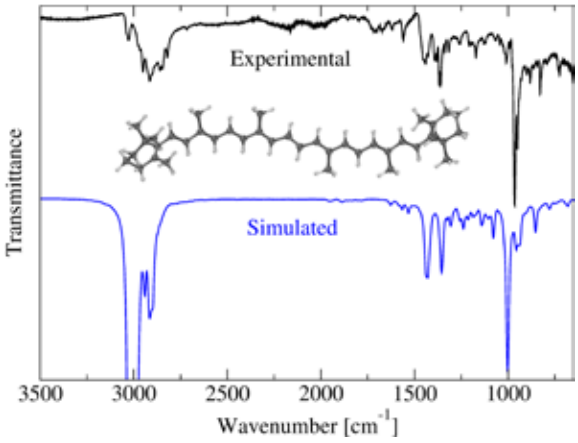


Fig. 1: Experimental and simulated IR spectra of β-carotene obtained from MD at HF-3c level of theory. The simulated spectrum has been scaled with a factor of 0.81.

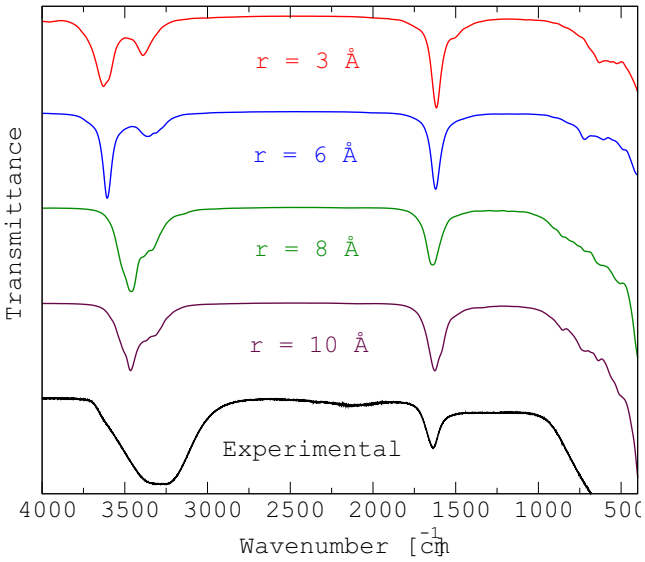


Fig. 2: Experimental IR spectrum of liquid water and simulated IR spectra of a central water molecule in four different water spheres (with radii 3 Å, 6 Å, 8 Å, and 10 Å containing 5, 41, 92, and 171 molecules, respectively) obtained from MD at HF-3c level of theory. The simulated spectra have been scaled with a factor of 0.81.

■ **L. D. M. Peters, J. Kussmann, C. Ochsenfeld:** *Efficient and Accurate Born-Oppenheimer Molecular Dynamics for Large Molecular Systems;* J. Chem. Theory Comput., 13, 5479 (2017).

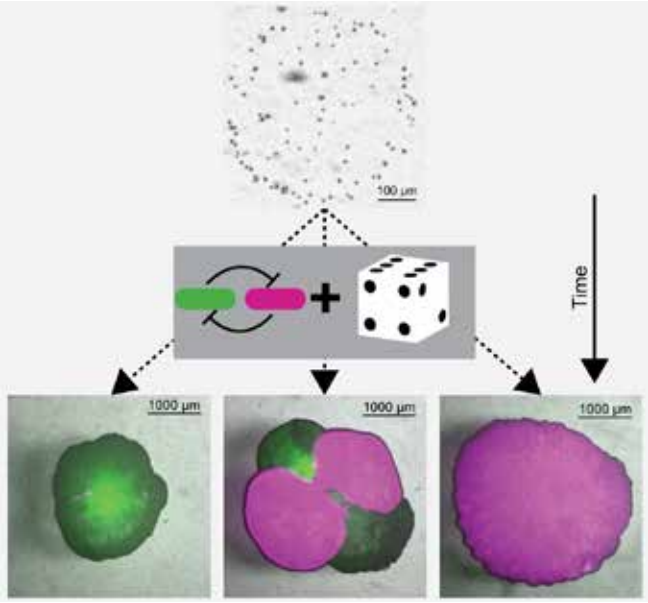
28

EFFECTS OF STOCHASTICITY AND DIVISION OF LABOR IN TOXIN PRODUCTION ON TWO-STRAIN BACTERIAL COMPETITION IN ESCHERICHIA COLI

PD Dr. Madeleine Opitz (LMU München, Physics Department)

■ www.softmatter.physik.lmu.de/personen/senior_scientists/opitz/index.html

Bacterial interactions determine microbial community composition dynamics, which in turn affects human physiology and human health. One important type of bacterial interaction is the competition by toxin release. Bacteriocins such as ColicinE2 produced by the bacterium *Escherichia coli* are toxins that are effective against closely related bacteria competing for the same resources. Many of these toxins are produced heterogeneously, so only a particular fraction of the bacterial population actually releases the toxin. For ColicinE2 it was shown that the type of toxin expression changes in dependence of the external stress level, shifting the population from only few producers that release the toxin stochastically with time to a population in which all cells produce and release the toxin early in a synchronous way. In the work of Bronk *et al.*, the researchers show that the degree of heterogeneous toxin production highly affects the competition of the toxin producing strain C with a strain sensitive towards the toxin. Furthermore, by combining experimental and theoretical approaches they demonstrate that stochasticity in toxin expression in the initial phase of the competition determines competition outcome. In particular, they observe that competitive success of the toxin producing strain (C) is only found if (i) a C edge cluster hast formed at the end of the initial competition phase and (ii) the beneficial and detrimental effects of toxin production are balanced, which is the case at intermediate toxin producer fractions. These findings highlight the importance of stochastic processes for bacterial competition, which might also be relevant for other microbial community interactions in which the random choice between phenotypes can have long-lasting effects for community fate.



■ **B. v. Bronk, S. A. Schaffer, A. Goetz and M. Opitz:** *Effects of Stochasticity and Division of Labor in toxin Production on Two-strain Bacterial Competition in Escherichia coli;* Plos Biology, doi.org/10.1371/journal.pbio.2001457 (2017).

29

FROM PRECURSOR POWDERS-TO-$CsPbX_3$ PEROVSKITE NANOWIRES: ONE-POT SYNTHESIS, GROWTH MECHANISM AND ORIENTED SELF-ASSEMBLIES

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Perovskite nanocrystals (NCs) have attracted great scientific and technological attention for their use in photovoltaics as well as in light emitting applications such as LEDs and lasers. They exhibit extremely high photoluminescence quantum yields reaching almost 100% and their emission color is easily tunable across the entire visible spectrum either by halide ion composition or or through their size. In spite of the rapid progress in the field of perovskite NCs, their growth mechanisms and morphology-dependent optical properties have not been well understood.

In this project, a facile one-pot synthesis approach for obtaining single-crystalline $CsPbBr_3$ perovskite nanowires (NWs) directly from the corresponding precursors by ligand-assisted dissolution and recrystallization under ultrasonication is demonstrated. The optical and morphological evolution revealed that the initially formed $CsPbBr_3$ nanocubes gradually transformed into NWs through an oriented-attachment mechanism. The emission color of the NWs can be tuned through the visible spectrum (400–680 nm) by varying the halide (Cl, Br, and I) composition through a subsequent halide ion exchange reaction. These perovskite NWs exhibit strongly polarized emission with a polarization anisotropy of 0.36. Interestingly, these NWs can be brought to spontaneously self-assemble into quasi-oriented assemblies at the air-liquid interface. This work not only provides a facile single-step method to synthesize highly monodisperse perovskite NWs, but also expands our current understanding of the growth mechanism and morphology-dependent optical properties and opens new avenues for the fabrication of highly ordered and oriented architectures using perovskite NC building blocks for future optical and optoelectronic devices.

■ **Y. Tong, B. J. Bohn, E. Bladt, K. Wang, P. Müller-Buschbaum, S. Bals, A. S. Urban, L. Polavarapu, J. Feldmann:** *From Precursor Powders-to-$CsPbX_3$ Perovskite Nanowires: One-pot Synthesis, Growth Mechanism and Oriented Self-assemblies;* Angew. Chem. Int. Ed., 56 (44), 13887-13892 (2017).

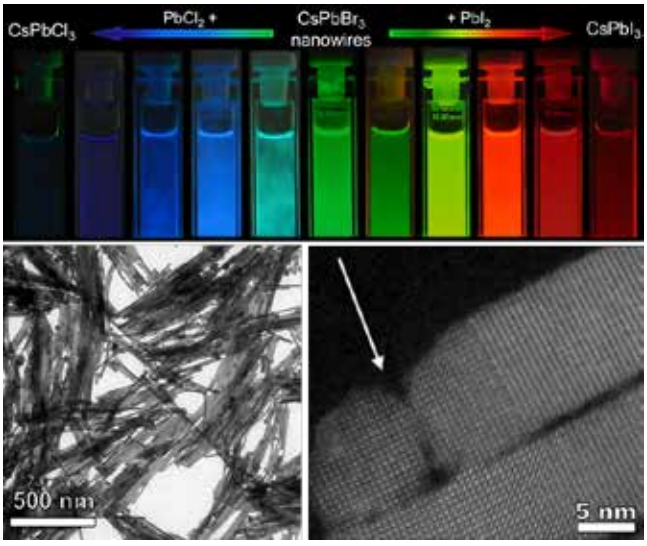

Fig. 1: The optical properties of perovskite nanowires are easily tunable across the entire visible spectrum by varying the halide composition though ion exchange reactions. The nanowires are uniform in thickness with lengths ranging from 500 nm to 2 μM. The nanowires are formed through the oriented-attachment of the initially obtained nanocubes in the reaction medium.

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MICROFLUIDIC SELF-ASSEMBLY OF FOLATE-TARGETED MONOMOLECULAR siRNA-LIPID NANOPARTICLES

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■ www.softmatter.physik.lmu.de
Prof. Ernst Wagner (LMU München, Department of Pharmacy)
■ www.cup.uni-muenchen.de/pb/aks/ewagner/

Nucleic acid particles for therapies based on RNA interference need to be small, stable and functional in terms of selective cell uptake and controlled release. In a joint project of the Rädler and Wagner group a rational design for optimal self-assembly of lipid-siRNA nanoparticles based on hydrodynamic mixing was developed. We created small (38 nm) monomolecular nucleic acid/lipid particles (mNALPs) that contain single molecules of short double-stranded oligonucleotides covered by a tight, highly curved lipid bilayer. The particles consist of DOPE, DOTAP, DOPC and DSPE-PEG(2000) and are assembled with 21 bp double-stranded DNA or small interfering RNA by solvent exchange on a hydrodynamic-focusing microfluidic chip. In comparison to vortex mixing by hand this method increases the encapsulation efficiency by 20%, and yields particles with a narrower size distribution, negligible aggregate formation and high stability in blood plasma and serum. Modification of mNALPs with folate-conjugated PEG-lipids results in specific binding and uptake by epithelial carcinoma KB cells overexpressing folate receptors. Binding is significantly reduced by competitive inhibition using free folate and is not observed with non-targeted mNALPs, revealing high specificity. The functionalized mNALPs show gene silencing in the presence of chloroquine, an endosome-destabilizing agent. The robust self-assembly of small-sized mNALPs with high stability and receptor-specific cell uptake may proof a promising approach towards improved delivery of short double-stranded oligonucleotides to living cells.

■ **R. Krzysztoń, B. Salem, D. J. Lee, G. Schwake, E. Wagner, and J. O. Rädler:** *Microfluidic Self-Assembly of Folate-Targeted Monomolecular siRNA-Lipid Nanoparticles;* Nanoscale 19, 60. doi:10.1016/j.biomaterials.2012.03.038 (2017).

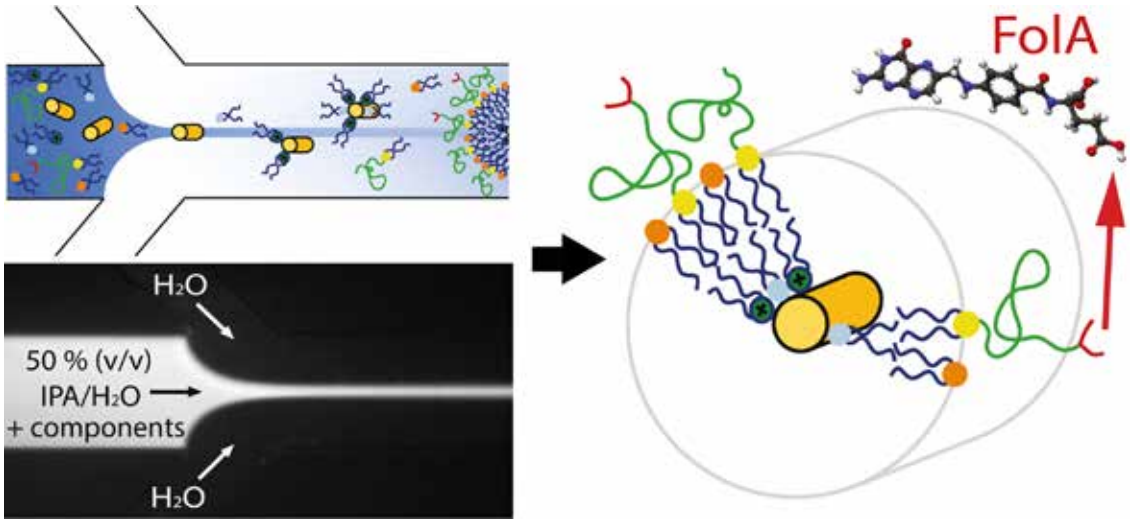

Fig. 1: The structure (right) and assembly of mNALPs in a microfluidic T-junction chip (left). Mixing at the nanoliter scale in microfluidic channels leads to rapid changes in solvent properties that drive particle formation.

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RECONSTITUTION OF PROTEIN GRADIENT OSCILLATIONS IN ARTIFICIAL MEMBRANE COMPARTMENTS

Prof. Petra Schwille (MPI of Biochemistry) ■ www.biochem.mpg.de/en/rd/schwille

The MinCDE protein machinery, wich orchestrates the positioning of the division ring in *E.coli* bacteria, shows a distinct oscillation of protein concentrations between the two cell poles, which are based on self-organization through reaction-diffusion. We have been able to reconstitute these self-organized oscillations of purified proteins in artificial cell-shaped compartments, as well as the faithful downstream positioning of protofilaments of the Z division ring. This could be the first step towards autonomous division of an artificial cell system, which we aim to establish in a bottom-up synthetic biology approach. Our research in the past year has been continuously devoted to quantitatively analyzing the biophysical and biochemical design features of this very simple and archetypical kind of a biological oscillator. Besides biochemical modifications to the Min proteins underyling the oscillator, we designed, together with our CeNS collaborators, an optical control system based on a light-switchable inhibitor, which allows us to tune the key oscillation features externally.

■ S. **Kretschmer, K. Zieske, P. Schwille:** *Large-scale modulation of reconstituted Min protein patterns and gradients by defined mutations in MinE's membrane targeting sequence;* PLoS ONE 12, e0179582 (2017).

P. Glock, J. Broichhagen, S. Kretschmer, P. Blumhardt, J. Mücksch, D. Trauner, P. Schwille: *Optical Control of a Biological Reaction-Diffusion System;* Angew Chem Int Ed., doi: 10.1002/anie.201712002. (2018).

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DNA NANOSTRUCTURES FOR SINGLE-MOLECULE SENSING OF ZIKA-SPECIFIC NUCLEIC ACIDS

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Infectious diseases are still the second leading cause of death in the world. A fast and direct detection of pathogens is often limited by a low signal-to-background ratio making molecular multiplication necessary. To tackle this problem, the group of Philip Tinnefeld used DNA origami nanostructures to develop a single-molecule detection method based on plasmonic fluorescence enhancement with optical nanoantennas and exemplified its functionality by detecting Zika virus nucleic acids. Plasmonic effects between light and metallic nanoparticles result in an electric field enhancement around the particle and hence, in a boosted fluorescence signal, if a dye is placed in this near field. The target nucleic acids are sensed by a DNA hairpin equipped with a fluorophore and a quencher. Only in the presence of specific target, the hairpin is opened and a fluorescence signal is generated. First it was shown that careful design of the fluorophore / quencher arrangement allowed synergistic signal generation by unquenching and a plasmonic fluorescence enhancement (Vietz et al.). For the molecular diagnostic assay, a silver nanoparticle was bound in a close proximity to the sensing unit resulting in an enhanced fluorescence upon target binding (Ochmann et al.). It was shown that already two single-nucleotide variations have an impact on the opening of the hairpin leading to a reduction from ~50% of opened hairpins to ~15% underlining its specificity. The functionality of this assay was further tested by using RNA as a target and by enriching heat inactivated human serum with target DNA. It could be shown that in both scenarios an increased signal is achieved as the hairpin was successfully opened by the targets. Also, by color barcoding the ability for the simultaneous detection of different targets was demonstrated. All in all, this work introduces a simplified detection method using DNA nanostructures opening the way for using low-tech detection devices and therefore making a step towards point-of-care diagnostics.

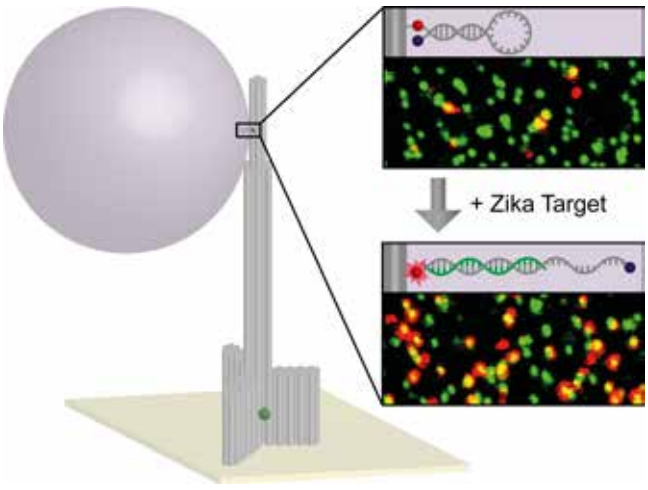

Fig. 1: DNA origami nanoantenna for signal amplification in fluorescence assays. The opening of the DNA hairpin by binding a Zika-virus specific nucleic acid releases the dye (red dot) from the quencher (dark blue dot) and more fluorescent red spots appear. The signal of the dye is further enhanced by the presence of the silver nanoparticle.

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SELF-ORGANIZATION OF ACTIN NETWORKS BY MONOMERIC MYOSIN MOTORS

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Specialised monomeric myosin motor proteins can induce the formation of extended actin lattice structures. Myosin class IX plays a critical role in acto-myosin networks that are required for cell polarisation and collective cell migration during morphogenesis and development. By combining quantitative super-resolution fluorescence microscopy, fluorescence spectroscopy and single particle electron microscopy the authors discovered that myosin-IX assembles actin filaments into highly ordered lattices. The polarity of the actin filaments is regulated by the motor protein itself. The actin filaments are connected by myosin-IX in a number of distinct structural conformations and at a repeat distance of precisely 36 nm across the network. The actin lattices induced by myosin-IX introduce orientated tracks with regularly spaced platforms for localised protein signalling activity during cell polarisation and collective cell migration.

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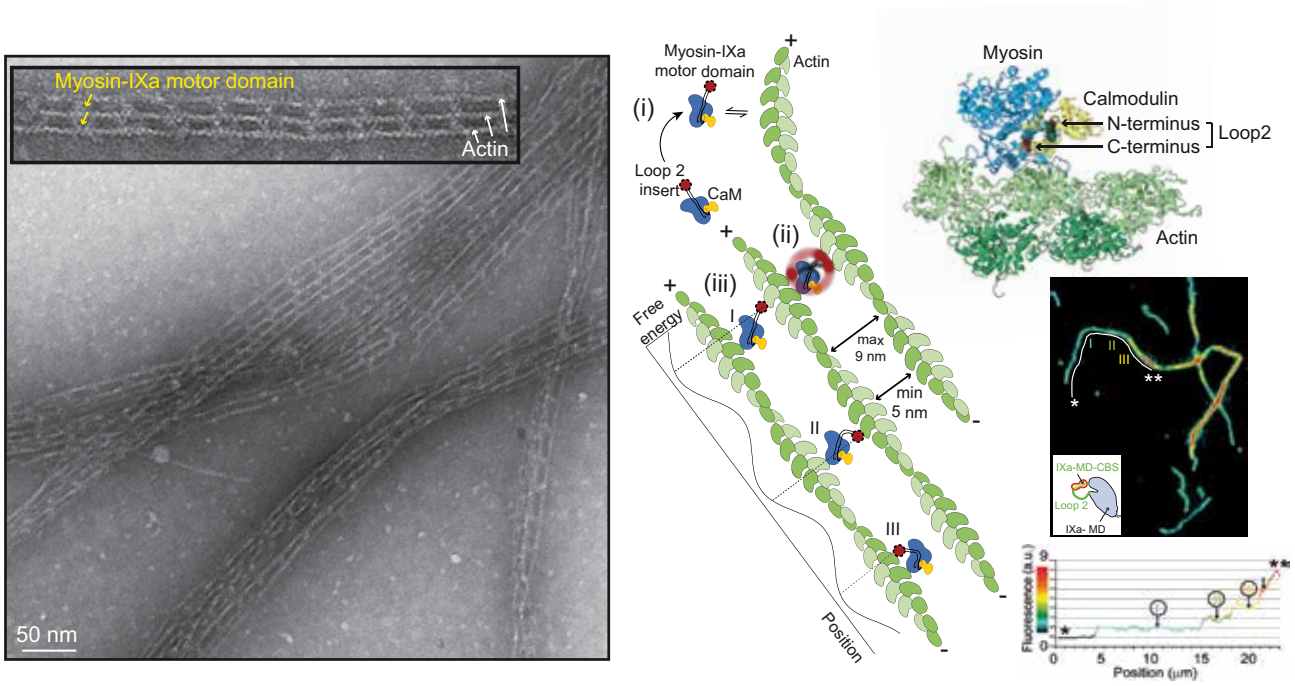

Fig. 1: Actin lattices induced by a monomeric myosin. The molecular motor myosin class IX (with its unique flexible insert (red) at the catalytic domain (blue)) can induce the formation of extended actin lattices by forming crosslinks between filaments with parallel polarity. The polarity of the filaments can be regulated by the motor. The motor can adopt three different conformations, crosslinking two filaments (I, II) or binding in an inchworm fashion to a single filament (III). In the inchworm conformation the motor can translocate along a single filament. This is the first demonstration of actin lattices induced by a monomeric motor of the cytoskeleton. The lattices introduce orientated tracks with regularly spaced platforms for localised protein signalling activity during cell polarisation and collective cell migration.

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SURFACE-MEDIATED CRYSTALLIZATION OF ORGANIC SEMICONDUCTORS FOR FIELD-EFFECT TRANSISTORS WITH HIGH ELECTRON MOBILITIES

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Deterministic crystallization of small organic molecules is essential for many fields of research and still poorly understood. Controlling the shape and structure of organic crystals by straightforward methods would clearly be a major step ahead towards actual applications of corresponding materials. For example, in the field of organic electronics, the quality and polymorphic form of crystalline thin films determines their electrical performance. In the present work, significant advancement towards truly deterministic crystallization of organic semiconductors has been made. More specifically, it was identified that the surface tension is the main driver for controlled two-dimensional crystallization of small organic molecules at the liquid-air interface, yielding highly crystalline thin films (see Figure). The crystallization process has been demonstrated using a novel air-stable perylene diimide of which only one monolayer thin, highly crystalline thin films have been deposited. Field-effect transistors using 3 nm thin films as semiconducting channel showed record mobilities of above 4 cm^2/Vs. This is one of the highest electron mobilities measured from solution deposited thin films and is especially remarkable given the extreme thinness of the organic semiconducting film.

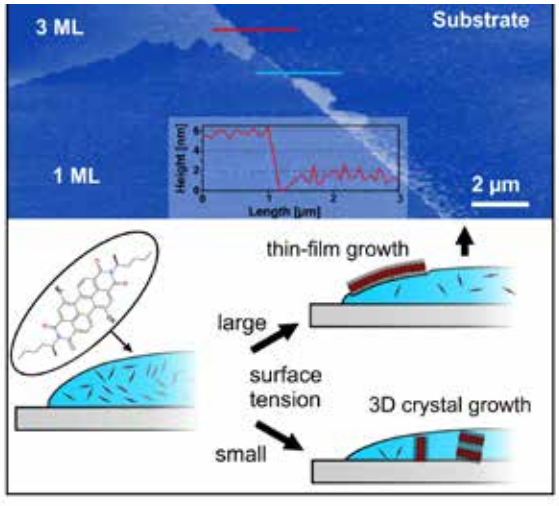

Fig. 1 (Bottom): Schematic of crystallization process: While solvents with a large surface tension and viscosity are found to promote thin film growth of the perylene diimide small molecule shown in the inset, solvents with small viscosity and surface tension lead to bulky crystals. **(Top):** Atomic-force microscopy image of a thin perylene diimide film crystallized from a high-viscosity solvent showing highly-crystalline, organic thin films that can be as thin as only one monolayer.

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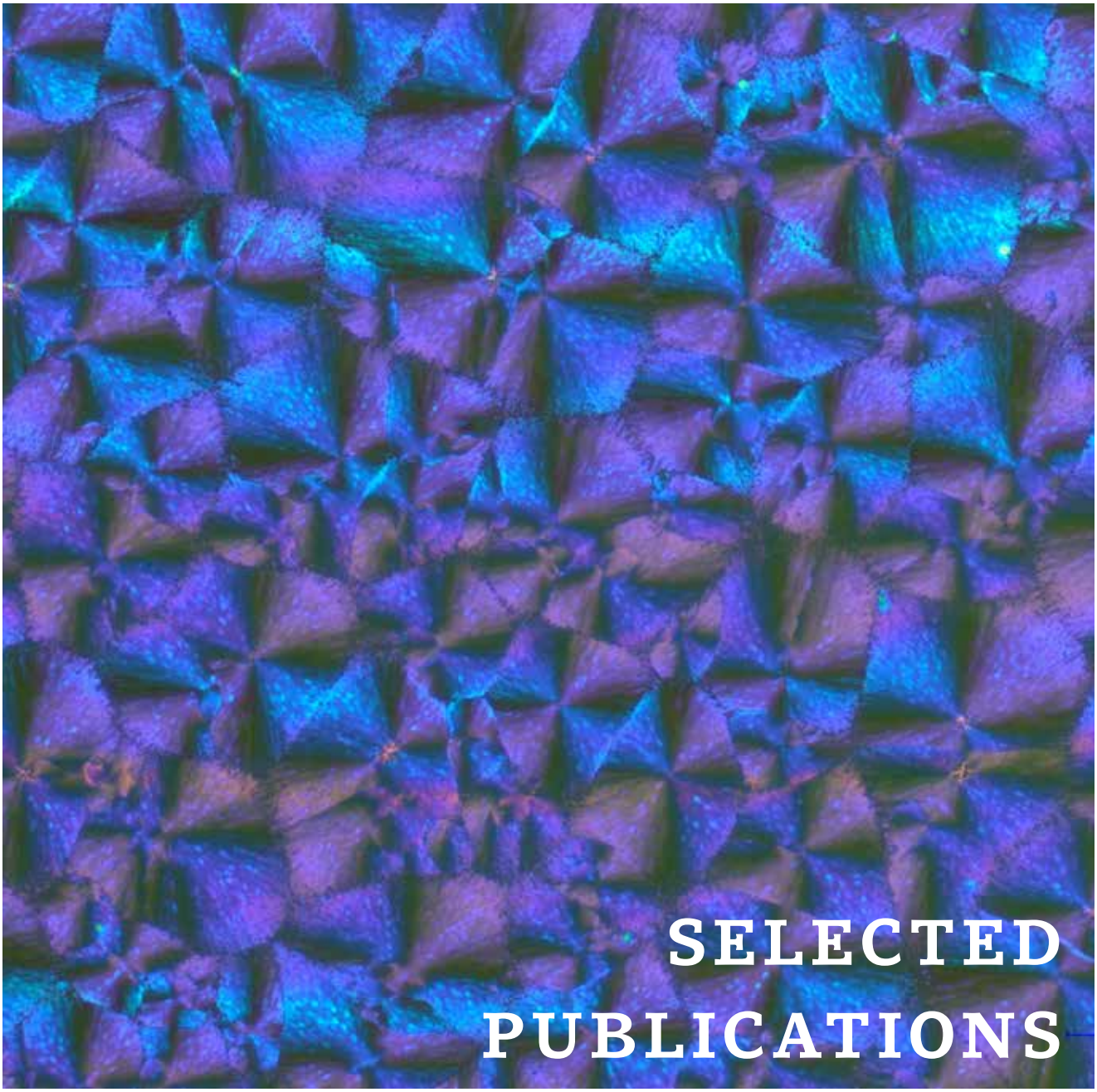

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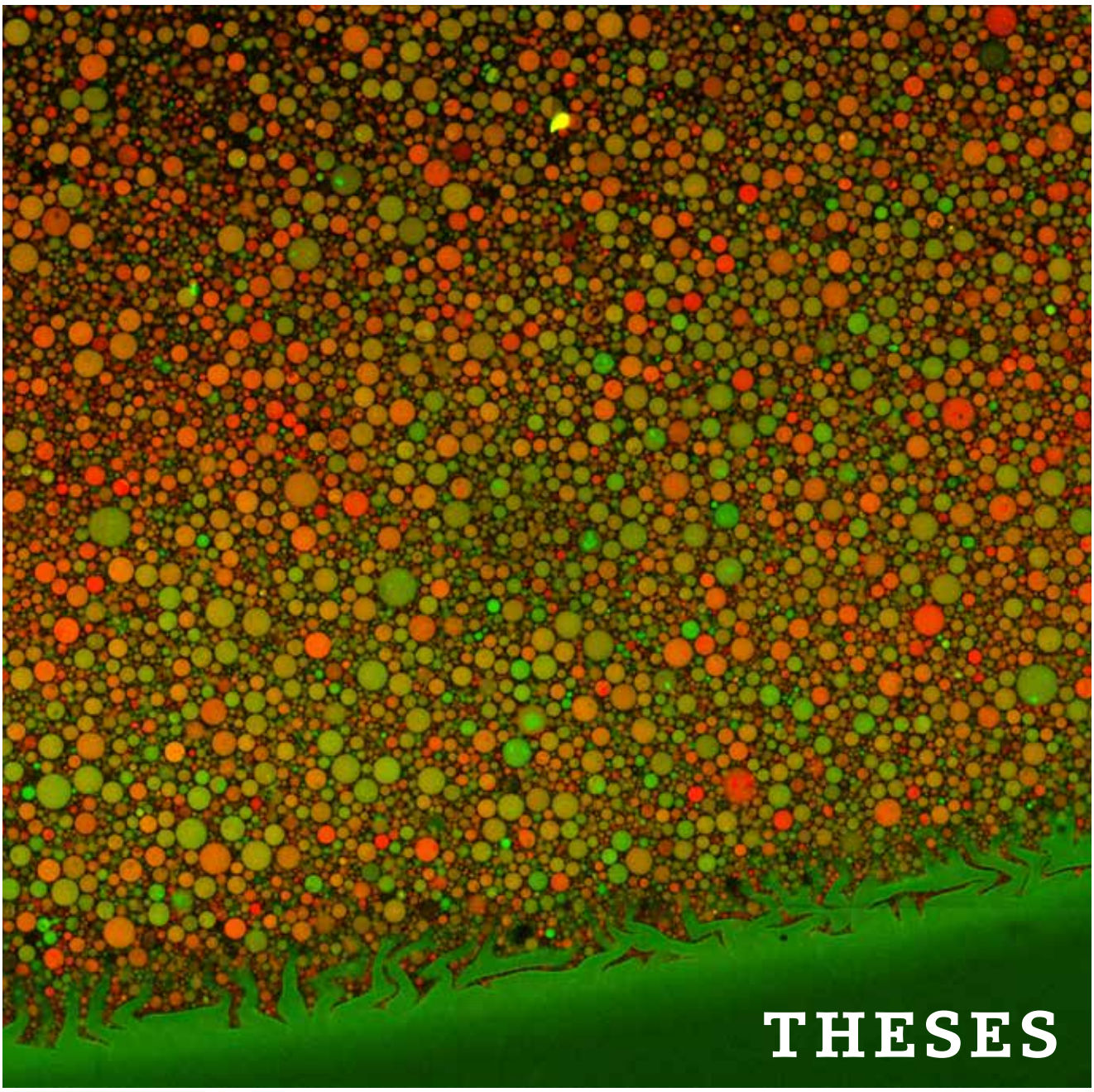
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Page 18, 19: private photographs
Page 21: Daniel Böhm, LMU
Page 59: Florin Walter, Jakob Lenz and Thomas Weitz, LMU
Page 67: Thomas Litschel, MPI of Biochemistry


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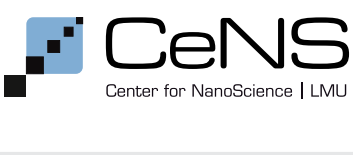
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