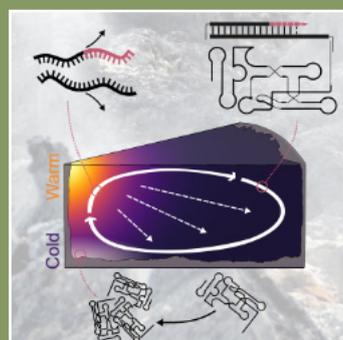
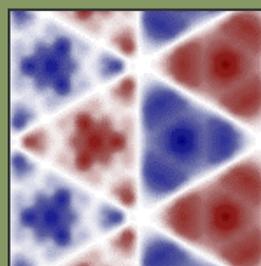
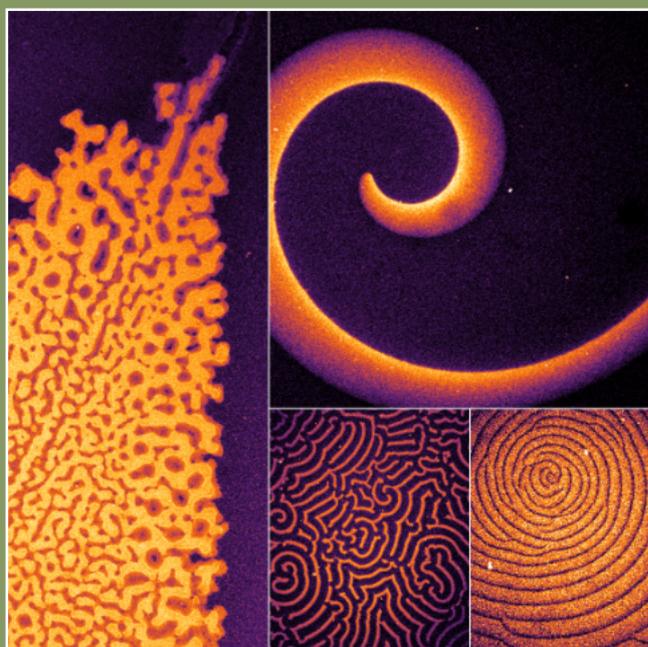


CENTER FOR NANOSCIENCE ANNUAL REPORT 2020



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WELCOME



We will certainly remember 2020 as a very challenging year, not only for all of us as individuals, but also for CeNS, our activities, plans, structure and functioning. However, with the enormous help of all of you and with the outstanding work by the CeNS

management team, Susanne Hennig and Claudia Leonhardt, we were able to adapt and to overcome the obstacles that the pandemic presented. Please join me here for an overview of the CeNS highlights during this difficult year.

Maybe one of the most obvious consequences of the pandemic was that we had to postpone most of our in-person activities in 2020, such as the CeNS-MCQST workshop in Venice, the CeNS winter retreat in Kleinwalsertal and the Junior Nanotech Network (JNN) exchange with the University of Cambridge. We are currently rescheduling some of these events for 2021/2022. However, we were able to restructure some of the other events in new formats, such as the online CeNS colloquium, which led to a great increase in the international audience and visibility. In addition, we were able to provide numerous online transferable-skills workshops for PhD students, especially during the first lockdown. Moreover, the online “CeNS meets Industry” event attracted more participants than in previous years, even without the traditional summer party!

There were changes in the CeNS Board. We extend our profound thanks to Prof. Tim Liedl and Prof. Claudia Veigel for their contribution over the years and we welcome Prof. Joachim Rädler and Prof. Emiliano Cortés, who joined the CeNS Board for the 2021-2022 period. We also welcome five new outstanding members who are introduced in detail later in this annual report: Amelie Heuer-Jungemann, Friedhelm Serwane, Olivia Merkel, Christine Papadakis and Leonardo de Souza Menezes from LMU, MPI of Biochemistry and TUM. With them, our CeNS family totaled 40 ordinary members plus 68 extraordinary members in 2020. Our next summer party is certainly going to be big! On the other hand, in 2020, we said farewell to Prof. Hermann Gaub, one of the founders of CeNS and

pioneers of the nano-bio-physics field at LMU. We are very grateful for his commitment and inspiration, and we wish him all the very best in this new stage of his life. We also said good-bye to Marilena Pinto, program manager at CRC1032 and well-known to the CeNS community. Thank you for your support, we will miss you, Marilena and Hermann! Throughout 2020, CeNS continued to support the career development and scientific ideas of its members by funding nine cooperation projects between CeNS groups, mostly involving young PIs and postdocs. Moreover, the extraordinary CeNS member Philipp Paulitschke founded the spin-off PHIO scientific GmbH in 2020. We are also very proud of and would like to congratulate some CeNS-related spin-offs - GNA Biosolutions, Ethris and Baseclick - that contributed to the fight against the pandemic by developing rapid Covid-19 tests and new therapeutics against the virus.

To finish, some more good news to celebrate. Despite the difficult year we all faced, CeNS members did an outstanding job securing funds for the coming years and receiving numerous prizes and awards. We would like to highlight and congratulate Dr. Amelie Heuer-Jungemann (MPI of Biochemistry) on her DFG Emmy Noether Grant; Prof. Ralf Jungmann (LMU & MPI of Biochemistry) on his ERC Consolidator Grant; Prof. Jan Lipfert (LMU) on his ERC Consolidator Grant; Dr. Friedhelm Serwane (LMU) on his ERC Starting Grant, and, last but not least, Dr. Andreas Tittl (LMU) on his DFG Emmy Noether Grant. Finally, the collaborative research center CRC1032 “Nanoagents” (spokesman: Prof. Rädler) secured funds for a third period (2021-2024). Congratulations to all of them!

We hope you will enjoy reading the CeNS annual report with all the very interesting and remarkable scientific contributions of CeNS members over the past year. Once more, we thank all of you for supporting and strengthening the CeNS network in these critical times, while we look forward to a fruitful and refreshing future.

Prof. Emiliano Cortés
Board Member of CeNS

NEW MEMBERS

DR. AMELIE HEUER-JUNGEMANN MPI of Biochemistry



Amelie Heuer-Jungemann is a research group leader at the Max Planck Institute of Biochemistry in Martinsried within the Department of Molecular Medicine. After studying Chemistry with Biochemistry at Heriot-Watt University in Edinburgh, she

then moved to the University of Southampton in 2011 to pursue a PhD in Physics (“Nanoparticle-DNA Conjugates for Biomedical Applications”). She subsequently received an EPSRC Doctoral Prize Fellowship allowing her to carry out independent research for one year as a postdoctoral fellow at the University of Southampton (2015-2016). Afterwards she took up a postdoctoral position at the LMU in the group of Tim Liedl (2016-2020). In 2020, she was awarded an Emmy Noether starting grant by the DFG. Her research group “DNA hybrid nanomaterials” uses DNA origami nanostructures to decipher complex cellular signaling cascades and investigates the interactions of DNA origami-templated silica nanostructures with cells for downstream biomedical applications as well as using such DNA-silica hybrid nanostructures for the creation of highly efficient enzyme cascades.

PROF. OLIVIA MERKEL LMU Munich



Olivia Merkel has been a Professor of Drug Delivery in the Department of Pharmacy at LMU Munich in Germany since 2015. From 2011 until 2017, she was an Assistant Professor of Pharmaceutics and an Associate Faculty

Member of Oncology at Wayne State University, Detroit, MI, USA, where she is also a Scientific Member of the Molecular Therapeutics Program and Faculty in the Cancer Biology Graduate Program at the Barbara Ann Karmanos Cancer Institute in Detroit, MI. She became a Registered Pharmacist in 2005. She received an MS in Pharmaceutics from Martin-Luther-Universität Halle-Wittenberg in 2006, and a PhD in Pharmaceutics from Philipps-Universität Marburg, Germany, in 2009. She has received several awards, including the PHOENIX award, the APV Research Award, Princess-Therese of Bavaria Award, an ERC Starting Grant, the Galenus Foundation Technology Award, the Young Investigator Award from the College of Pharmacy at Wayne State, the Young Pharmaceutical Investigator Award granted by the European Federation for Pharmaceutical Science, an invitation to the Lindau Nobel Laureates Meeting, the Carl-Wilhelm-Scheele-Award by the German Pharmaceutical Society (DPHG) and the award for the best PhD thesis at Philipps-Universität Marburg. From 2015 to 2017, Prof. Merkel headed research labs in both Detroit and Munich. Currently her research centers around targeted RNA delivery in cancer, inflammatory diseases and viral infections with a focus on pulmonary administration and is funded by the ERC, several foundations, Daiichi-Sankyo Europe, and AbbVie.

PROF. CHRISTINE PAPADAKIS TU Munich



Christine M. Papadakis is a professor at the Physics Department of Technical University of Munich and head of the Soft Matter Physics Group. After studying physics at the Universities of Mainz and Grenoble, she completed her doctorate at Roskilde University, Denmark. Following a postdoctoral stay (1996-98) at Risø National Laboratory, Roskilde,

Denmark, Prof. Papadakis earned her postdoctoral teaching qualification at the University of Leipzig in 2003. She has been a member of proposal committees at several large-scale facilities and is editor-in-chief of *Colloid & Polymer Science*, Springer Verlag. Her group uses light, X-ray and neutron scattering methods, also with complex sample environments (e.g. under high pressure or in controlled solvent vapor atmosphere) to investigate polymers of complex architecture, (multi-)responsive polymers, block copolymers and polymers for drug delivery. In time-resolved scattering experiments during rapid changes of temperature or pressure or during swelling of polymer films, the pathways of structural changes are determined.

DR. FRIEDHELM SERWANE LMU Munich



Friedhelm Serwane's research career is characterized by his curiosity about fundamental systems in various disciplines: after his doctorate in the field of ultracold quantum gases (Ruprecht-Karls-Universität Heidelberg), he

switched to biophysics as a postdoctoral researcher at the European Molecular Biology Laboratory in Heidelberg (2012-2013) and at the University of California, Santa Barbara (2013-2016). As a Feodor-Lynen postdoctoral fellow, he investigated the role of mechanics during embryonic development. He became intrigued by stem cell-derived neuronal systems (retina organoids), which he established as a project leader at the MPI for Medical Research in Stuttgart (2016-2018). During his work at Airbus' Central Research & Technology in the field of quantum sensing and communication (2019-2020), he gained experience in leading scientists at the interface between the university and industrial research. In September 2020, Dr. Serwane started his new ERC funded research group "ROMB: Retina Organoid Mechanobiology" at LMU Physics. He and his team will focus on a unique combination of biophysical methods and stem cell-derived systems (organoids).

PROF. LEONARDO DE SOUZA MENEZES LMU Munich



Leonardo de Souza Menezes studied Physics at the Institute of Physics, Universidade Federal do Rio de Janeiro, Brazil. After his Doctorate on nonlinear spectroscopy of organic molecules with incoherent light, he worked as an associate researcher on optical

fiber amplifiers based on Raman scattering and multiwavemixing processes. As an Alexander von Humboldt post-doc fellow, he researched on optical microcavities with ultrahigh quality factors at the Humboldt University Berlin. Back in Brazil, in 2005 he obtained a Professorship at the Physics Department/Universidade Federal de Pernambuco-UFPE (Recife-PE, Brazil), where he has been leading two research laboratories dedicated to nanooptics, applying various linear and nonlinear spectroscopic techniques in the study of single nanoparticles, quantum emitters in the presence of critical media, colloids and metasurfaces based on metallic nanoparticles and random lasing. Prof. Menezes spent a sabbatical year at the MPI for the Science of Light, working with Interferometric Scattering aiming at independently measuring the scattering and absorption cross sections of single nanoparticles. In 2020, Prof. Menezes joined the Chair in Hybrid Nanosystems - Faculty of Physics, LMU Munich as a subgroup leader, doing research on coherent mechanical oscillations of single metallic nanoparticles, the use of rare-earth doped dielectric single nanocrystals for thermometry with spatial resolution on the nanometer scale, new platforms for photonic microcircuits and light emission from quantum emitters.

MEMBERS' NEWS

CALLS & APPOINTMENTS



Prof. Alexander Holleitner accepted an offer as full professor W3 for Nanotechnology and Nanomaterials at TUM Physics Department and declined an offer for a W3 position at TU Berlin.



Prof. Hubert Krenner declined a call to Linz University and accepted a call as full professor (W3) for Experimental Physics at Münster University.



Dr. Hannes Mutschler was appointed full professor (W3) for Biomimetic Chemistry at TU Dortmund.



Dr. Lakshminarayana Polavarapu became PI at the Biomedical Research Centre, University of Vigo, Spain.

AWARDS & GRANTS



PD Dr. Tayebbeh Ameri (LMU) was awarded the Arnold-Sommerfeld-Prize of the Bayerische Akademie der Wissenschaften.



Prof. Thomas Bein (LMU) received the joint Elhuyar-Goldschmidt Award of the Spanish Royal Society of Chemistry and the German Chemical Society.



PD Dr. Hanna Engelke (LMU, now Universität Graz) won a Römer Preis for Junior Research Groups of the Faculty of Chemistry and Pharmacy.



Dr. Amelie Heuer-Jungemann (MPI of Biochemistry) received a DFG Emmy Noether Grant.



Prof. Ralf Jungmann (LMU & MPI of Biochemistry) was granted an ERC Consolidator Grant for his project "Receptor-PAINT – Imaging Receptomics as a tool for biomedical discovery".



Prof. Jan Lipfert (LMU) received an ERC Consolidator Grant for his project ProForce - Mechano-Regulation of Proteins at Low Forces: Paving the Way for Therapeutic Interventions. In addition, he won a triple - the 2020 teaching prizes of the Department of Biology, the Faculty of Physics, and the Faculty of Chemistry and Pharmacy.



Prof. Stefan Maier (LMU) was honored with the ACS Nano Lectureship Award.



Prof. Olivia Merkel (LMU) was awarded the APV Research Award for Outstanding Achievements in the Pharmaceutical Sciences and the PHOENIX Pharmazie Wissenschaftspreis.



Prof. Petra Schwille (MPI of Biochemistry) received the Carl Zeiss Lecture Prize 2020.



Dr. Friedhelm Serwane (LMU) was awarded an ERC Starting Grant for his project ROMB: Retina Organoid Mechanobiology.



Dr. Andreas Tittl (LMU) received an DFG Emmy Noether Grant.

CENS BOARD



Prof. Emiliano Cortés was elected as a new member of the CeNS board.



Prof. Joachim Rädler was elected as a new member of the CeNS board.

COLLABORATIVE RESEARCH

The **SFB 1032 "Nanoagents for Spatio-temporal Control of Molecular and Cellular Reactions"** secured funding for a third period. 22 groups, including 20 CeNS members are involved in this collaborative research center. Funding will run until June 2024.

AWARDS

NANO INNOVATION AWARD



On July 24, the Nano Innovation Award 2020 was presented by CeNS in the beautiful LMU Aula. Three graduate students from Würzburg and Munich received the award for

promising, application-oriented results as part of their thesis in nanosciences. The Bavarian-wide prize was endowed with €7,500 and was awarded by a jury of experts from science and business (Prof. Jens Rieger, Prof. Khaled Karrai, Prof. Hubert Krenner, Prof. Angelika Vollmar, Prof. Joachim Rädler).

In the last decades, nanoscientific research has led to many technical applications - with great economic impact. Therefore, the Nano Innovation Award focuses specifically on innovative work with promising application potential in technology or biomedicine by junior researchers in Bavaria.

Into the blue - perovskite nanocrystals for next-generation LEDs

The first prize, endowed with €3,500, went to Dr. Bernhard Bohn from the group of Prof. Jochen Feldmann at LMU Munich. His work constitutes a technological breakthrough in producing perovskite nanocrystal light emitters with an unprecedented quantum yield in the blue, a wavelength range that was not accessible previously in such systems. The results open up a very wide range of potential applications, for example by enabling white all-perovskite LEDs, a comparatively cost effective technology to implement. The success of the work is built on the scientific insight gained from understanding light emission dynamics in such nanostructures that in turn allowed an optimization of the nanocrystals towards the desired very high emission yield.

DNA Nanotechnology for sensitive diagnostics

Linh Nguyen from the group of Prof. Tim Liedl at LMU Munich was the winner of the second prize, endowed with €2,500. She came up with the ingenious but simple idea of a one-pot reaction to synthesize highly stable silver nanorods and nanoparti-



The Award Ceremony was livestreamed from the LMU Great Assembly Hall (Aula). From left to right: Jury member Khaled Karrai (attocube), jury member Joachim Rädler (CeNS), winner Bernhard Bohn, Amelie Heuer-Jungemann (supervisor of 2nd prize winner Linh Nguyen), 3rd prize winner Enno Krauss and CeNS spokesman Dieter Braun.

cles coated with a wide range of hydrophilic anchor groups, including DNA. Her method solves the long-standing problem that silver nanoparticles with any coating degrade fast in aqueous environments. Since silver is an excellent material for plasmonic studies and applications, this opens up a wide range of possible applications, for instance in diagnostics. Linh was able to produce impressive results with lateral flow assays in which her silver-coated particles provide higher detection sensitivity than standard gold nanoparticles. Linh Nguyen has already filed a patent application for her innovative approach, and she and postdoc Max Urban are currently working on commercializing their ideas by starting their own company.

Nano-Optics with single-crystal gold platelets

The third winner came from the group of Prof. Bert Hecht at the University of Würzburg: Enno Krauss developed a simple but clever method to optimize the manufacturing process of plasmonic nanostructures by making use of single-crystal gold platelets, enabling him to produce extremely precise arrays of gold wires. In the future, these results could open up a broad range of applications in nano-photonics and new applications in quantum information processing. Enno Krauss is part of a team that already has already received an EXIST grant for the start-up "NanoStruct", to bring their idea of commercial large-scale production of homogeneous metallic nanostructures to the next level.

CeNS awarded the Nano Innovation Award 2020 together with three companies that are originally spin-offs from CeNS: attocube systems, Nanion Technologies, and NanoTemper Technologies. "All three companies were born from the special blend of top science and technology that grew out of CeNS. The Nano Innovation Award aims at keeping that tradition alive, namely building bridges between science and technology on the topic of nano. It also helps to boost careers at the interface between the academic and industry worlds and brings awareness of the complementarity of both. Great science, but also entrepreneurial opportunities are the reward for our society." says Prof. Khaled Karrai, scientific director of attocube and member of the jury.

■ <https://www.youtube.com/watch?v=NMqMEF-nAlAo>

CENS PUBLICATION AWARDS

In 2021, CeNS awarded 10 prizes for excellent publications by CeNS members that were published during the past twelve months. Successful CeNS internal collaboration projects, such as those between the groups of Prof. Tim Liedl and Prof. Don Lamb or between Prof. Erwin Frey and Prof. Petra Schwille, were amongst those that received an award.

In addition, outstanding articles from individual research groups which were published in renowned journals such as Nature Methods and Phys. Rev. Lett. were recognized in the category "Scientific breakthrough". Last but not least, the junior CeNS members Hanna Engelke, Jacek Stolarczyk, Oliver Thorn-Seshold and Strefan Wuttke were honored for their publications.

All winning publications are highlighted in the "Selected publications" section of this report (page 53).

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

SPIN-OFF NEWS

BASECLICK

Baseclick GmbH received financial support from BORN2GROW to develop an mRNA-based vaccine to combat the COVID-19 pandemic. In addition, baseclick has developed a new and more efficient process to determine not only predominant mutations but also minor occurring mutations in a virus population which might eventually become new strains. The "Click Tech Single Strain Mutation Mapping Kit for Sars-Co-V2" together with "long-read" sequence methods, allows an exact genomic assignment and an assessment of the frequency of newly emerging virus variants in the population.

■ www.baseclick.eu

CHROMOTEK

ChromoTek, a manufacturer of Camelid, single-domain antibodies, also known as nanobodies, was acquired by Proteintech, in October 2020. The combined companies will better address the industry's growing opportunities and challenges in single cell analysis, super resolution imaging, and multiplex assays.

■ www.chromotek.com

ETHRIS

In April 2020, Ethris GmbH signed an exclusive partnership with Neurimmune AG to develop mRNA-encoded, neutralizing anti-SARS-CoV-2 antibodies administered by inhalation for the treatment of Covid-19. The collaboration brings together Neurimmune's expertise in developing human antibodies based on high-throughput immunoglobulin sequence analyses from Covid-19 patients who have recovered from the disease and Ethris' proprietary and unique pulmonary SNIM®RNA therapeutics platform. Both companies are working together to rapidly develop an immunotherapy designed to produce therapeutic antibodies directly in the lungs of affected patients.

www.ethris.com

GNA BIOSOLUTIONS

Molecular diagnostics startup GNA Biosolutions received Emergency Use Authorization from the German Federal Institute for Drugs and Medical Devices for the GNA Octea SARS-CoV-2 Test System. The new technology enables decentralized COVID-19 rapid tests in approximately 40 minutes without sacrificing sensitivity. The GNA Octea SARS-CoV-2 Test System is based on Pulse Controlled Amplification (PCA®) technology. The system is comprised of the GNA Octea portable analyzer and a SARS-CoV-2 test kit and performs rapid molecular detection of the SARS-CoV-2 virus from oropharyngeal swabs.

■ www.gna-bio.de

IBIDI

Ibidi's CEOs Dr. Valentin Kahl and Dr. Roman Zantl were recognized together in the ranking of the Top 25 Healthcare Technology CEOs of Europe for 2020. The nominees were evaluated based on the breadth and depth of their experience, their consistently high organizational performance, their contributions to the industry, and their reputation among their peers. Each of the CEOs recognized has had a profound impact on the companies they lead, including making strategic decisions to drive operational expansion, augmenting research capabilities, and launching new products and services..

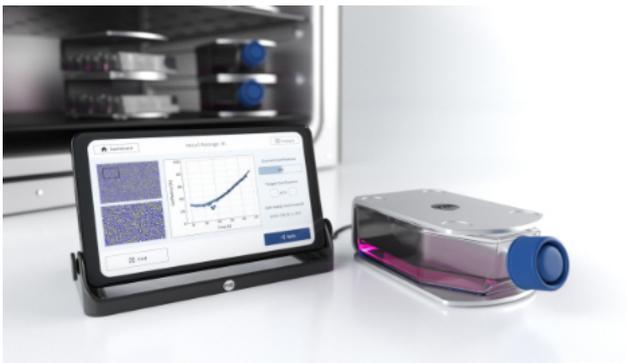
■ www.ibidi.com



PHIO

In March 2020, PHIO Scientific GmbH was founded by CeNS member Dr. Philipp Paulitschke. Phio's mission is to boost cell-based research. The super compact lensless PHIO microscope gives fully automatic imaging directly inside the incubator. The system is connected to a cutting-edge AI analysis platform and facilitates cell motility studies, drug screening, cell culture quality control, tracking cell fitness over passages and more - just by setting the microscope running and letting it send the finished data.

■ www.phio.de



QLIBRI

The pre-startup Qlibri received the prestigious EX-IST Forschungstransfer start-up grant from the German Federal Ministry for Economic Affairs and Energy (BMWi). Their products use optical microresonators to enhance the interaction between light and matter at the nanoscale. In 2020, the team behind Qlibri, Dr. Thomas Hümmer and Dr. Jonathan Noé, managed to record a complete hyperspectral microscopy image with the noise floor well below 0.001% recorded in less than a second for the first time.

■ <https://qlibri.eu/>

DEOXY



In September 2020, the DEOXY team ranked third in the largest business plan competition in Germany. The independent start-up initiative Science4Life e.V. organizes the business plan competition for the life sciences, chemicals and energy sectors once a year. The research team led by CeNS members Johannes Wöhrstein and Heinrich Grabmayr is developing a platform technology that can be used to quickly and reliably measure the activity of genes in individual cells in a high-throughput process. To do this, they are using specially developed fluorescent nanoparticles that allow them to visualize and count the number of messenger RNA molecules (mRNAs) of a known gene. The direct detection of known genes makes the DEOXY system precise and highly sensitive, making it interesting for clinical practice.

■ <https://deoxy.bio/>

EVENTS & ACTIVITIES

2020 brought special challenges for the Center for NanoScience. In March, the winter retreat in Kleinwalsertal had to be cancelled due to the rapid spread of the corona virus. Later, it also became clear that other events, such as the Venice workshop, the Annual Assembly or CeNS meets Industry, would have to be cancelled or take place online.

For the weekly CeNS colloquium, the webinar format became quite successful, attracting attendees from CeNS but also the international research community, with the participants outnumbering those in the previous on-site seminars.

In the winter term, the student-organized seminar series “Science Rocks!” went online, too. The organizers invited junior scientists from different CeNS labs who presented their COVID-19 related research.

CENS @HOME

In spring 2020, when “social distancing” and lockdown were still new concepts, the life of many PhD students changed drastically. Labs were closed or only open to a limited number of people.

Seminars, conferences and workshops had to be cancelled. During this strange time, CeNS quickly developed a four-week online program to support the CeNS associates in this challenging situation and to allow for social interaction. The program aimed to foster a feeling of community, offering virtual spaces conducive to learning, reflection and group discussion. Each week focused on a different aspect, offering workshops and seminars on topics such as time management and staying motivated at home, communication in science, career development, and research integrity.

In the following months, this condensed program was complemented with further online workshops on topics such as Entrepreneurship & Innovation, project management for scientists, or getting published and mastering peer-review, which attracted many participants.

CENS MEETS INDUSTRY

In 2020, career networking opportunities for junior scientists were limited considerably by the pandemic, lending special significance to “CeNS meets Industry”. On the other hand, the virtual format allowed CeNS to go bigger – more talks, more participants, and more participating companies. The plenary lecture was held by Prof. Sebastian Springer, Jacobs University Bremen, who provided interesting insights into immunoprotein arrays for basic science and medical diagnosis. In two parallel sessions, representatives and alumni from industry and various business sectors presented diverse career paths and employment opportunities to the junior scientists of CeNS – ranging from large companies such as Eurofins, Zeiss, Siemens, or Google to local ones such as GNA Biosolutions or Molecular Machines and Industries. The subsequent company fair was well-attended, giving the opportunity for one-to-one conversations with the invited speakers. Despite the numerous advantages of the online format, the CeNS community missed the annual CeNS summer party as the perfect opportunity for networking and exchange.

FOCUS WORKSHOP

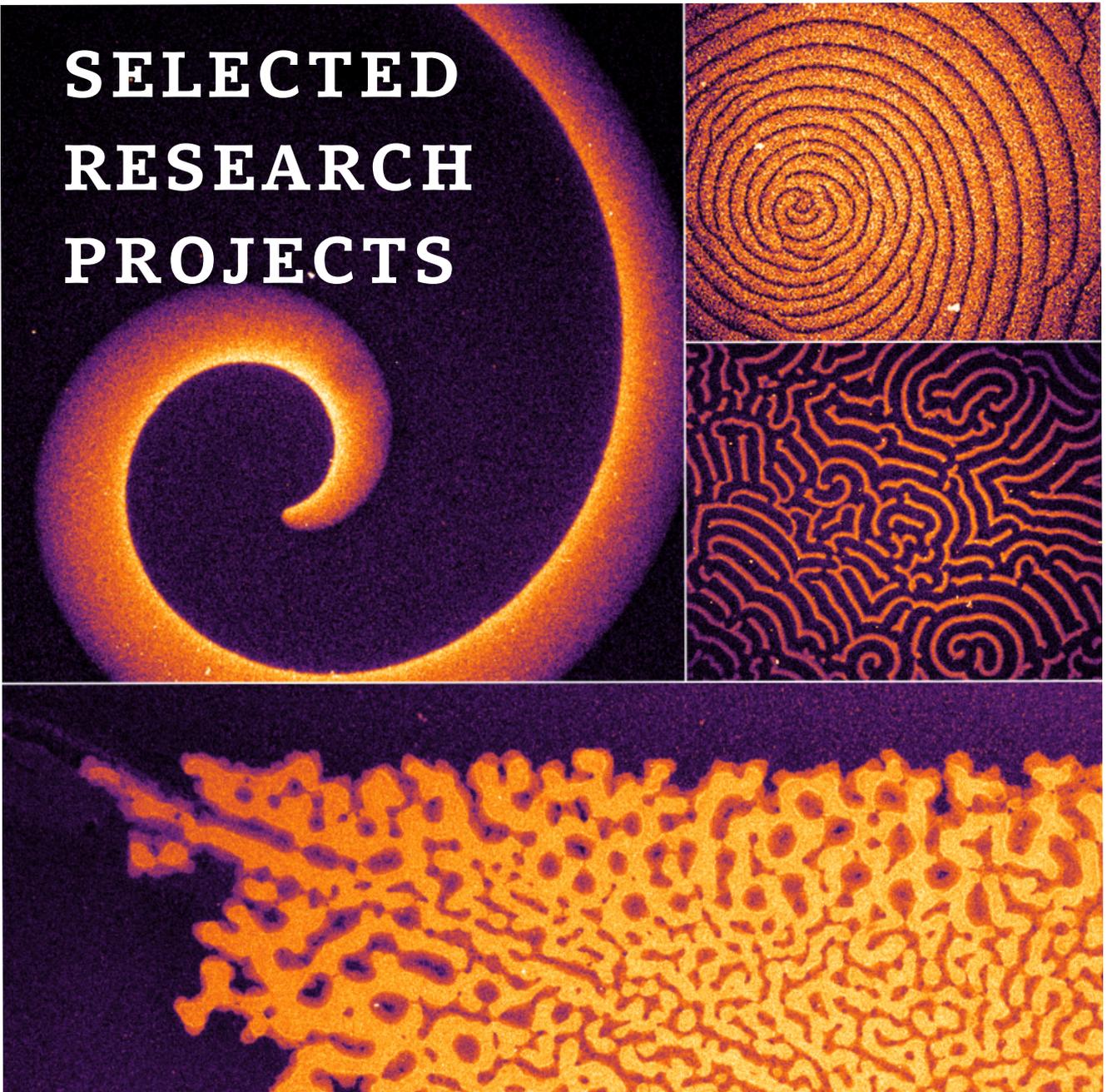


The 4th Functional DNA Nanotechnology Workshop was held in Rome from October 7 to 9, 2020.

Despite the pandemic, the organizers Tim Liedl (CeNS) and Francesco Ricci (University of Rome, Tor Vergata) succeeded in setting up a live event with 65 participants, financially supported by CeNS. The scope of the workshop was to share knowledge and ideas about functional DNA nanotechnology (nanostructures, DNA origami, etc.), bioengineering, synthetic biology, DNA-based sensing, aptamers, and DNA-peptide chimera..

■ <http://www.fdn2020.com/>

**SELECTED
RESEARCH
PROJECTS**



SELECTED RESEARCH PROJECTS

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■ <https://bein.cup.uni-muenchen.de>

■ <https://www.groups.ph.tum.de/en/polymer/peter-mueller-buschbaum>

Lead-free double perovskites have recently attracted growing attention as possible alternatives to lead-based halide perovskites in photovoltaics and other optoelectronic applications. The most prominent compound $\text{Cs}_2\text{AgBiBr}_6$, however, presents issues such as a rather large and indirect band gap, high exciton binding energies, and poor charge carrier transport, especially in thin films. In order to address some of these challenges, the group systematically modified the stoichiometry of the precursors used for the synthesis of thin films toward a BiBr_3 -deficient system. In combination with a stoichiometric excess of AgBr , they obtained highly oriented double perovskite thin films. These modifications directly boost the lifetime of the charge carriers up to 500 ns as observed by time-resolved photoluminescence spectroscopy. Moreover, time-resolved microwave conductivity studies revealed an increase of the charge carrier mobility from 3.5 to around similar to $5 \text{ cm}^2/(\text{V s})$. Solar cells comprising the

modified films as planar active layers reached power conversion efficiency (PCE) values up to 1.11%, exceeding that of the stoichiometric reference film (0.97%), both on average and with champion cells. The results of this work underline the importance of controlling the nanomorphology of the bulk film. The group anticipates that control of precursor stoichiometry will also offer a promising approach for enhancing the efficiency of other perovskite photovoltaic absorber materials and thin films.

■ M. T. Sirtl, M. Armer, L. K. Reb, R. Hooijer, P. Dörflinger, M. A. Scheel, K. Tvingstedt, P. Rieder, N. Glück, P. Pandit, S. V. Roth, P. Müller-Buschbaum, V. Dyakonov, and T. Bein: *Optoelectronic Properties of $\text{Cs}_2\text{AgBiBr}_6$ Thin Films: The Influence of Precursor Stoichiometry*; ACS Applied Energy Materials 3, 11597 (2020).

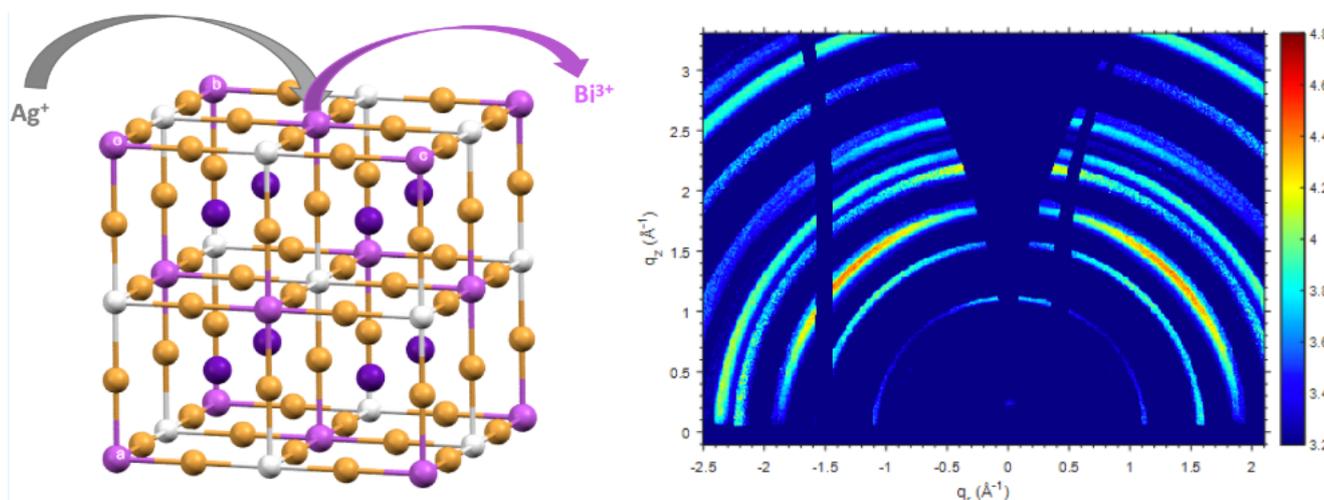


Fig. 1. Left: Structure of the lead-free double perovskite $\text{Cs}_2\text{AgBiBr}_6$. Right: GIWAXS data of a thin film of $\text{Cs}_2\text{AgBiBr}_6$ with BiBr_3 deficiency, combined with AgBr excess (1.15:0.85; 15 mol %).

HOW PHOTOCORROSION CAN TRICK YOU: A DETAILED STUDY ON LOW-BANDGAP LI DOPED CuO PHOTOCATHODES FOR SOLAR HYDROGEN PRODUCTION

Jonathan Kampmann, Sophia Betzler, H. Hajiyani, Sebastian Häringer, Michael Beetz, T. Harzer, J. Kraus, Bettina V. Lotsch, Christina Scheu, Rossitza Pentcheva, Dina Fattakhova-Rohlfing, and Thomas Bein

■ <https://bein.cup.uni-muenchen.de/>

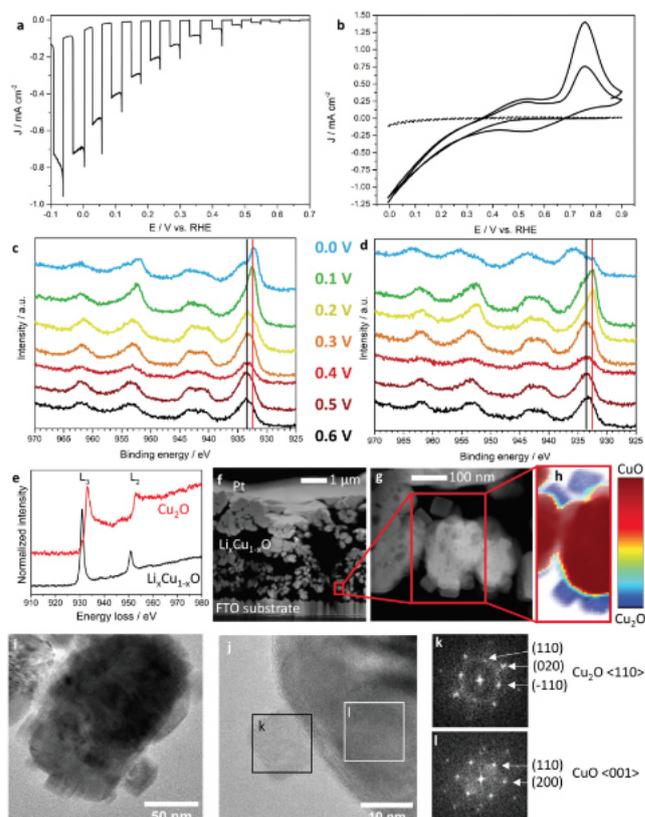
■ https://www.fz-juelich.de/iek/iek-1/EN/Research/Department_ElectrochemicalStorage

■ <https://www.fkf.mpg.de/lotsch>

The efficiency of photoelectrochemical tandem cells is still limited by the availability of stable low band gap electrodes. In this collaborative project between several CeNS groups, the authors report a photocathode based on lithium doped copper(II) oxide, a black p-type semiconductor. Density functional theory calculations with a Hubbard U term show that low concentrations of Li ($\text{Li}_{0.03}\text{Cu}_{0.97}\text{O}$) lead to an upward shift of the valence band maximum that crosses the Fermi level and results in a p-type semiconductor. Therefore, Li

doping emerged as a suitable approach to manipulate the electronic structure of copper oxide-based photocathodes. As this material class suffers from instability in water under operating conditions, the recorded photocurrents are often misinterpreted as hydrogen evolution evidence. The group investigated the photocorrosion behavior of $\text{Li}_x\text{Cu}_{1-x}\text{O}$ cathodes in detail and provided the first mechanistic study of the fundamental physical process. The reduced copper oxide species were localized by electron energy loss spectroscopy

Fig. 1. (a) Linear sweep voltammogram of a bare $\text{Li}_x\text{Cu}_{1-x}\text{O}$ film under chopped AM 1.5 illumination, showing no signs of photocorrosion. The assumption of a working photocathode based on this experiment is misleading, as the reductive currents originate from both water reduction and photocorrosion. (b) Cyclic voltammetry characterization of an unprotected $\text{Li}_x\text{Cu}_{1-x}\text{O}$ photocathode in 0.1 M Na_2SO_4 at pH 7 in the dark (dashed line) and under AM 1.5 illumination through the substrate (solid line). (c and d) Cu 2p XPS spectra measured of bare $\text{Li}_x\text{Cu}_{1-x}\text{O}$ films held at the respective potentials vs. RHE for 15 minutes each in the dark (c) and under AM1.5G illumination (d) (bars: black: Cu^{2+} , red: Cu^0 and Cu^{1+}). At a potential of 0.2 V vs. RHE, $\text{Li}_x\text{Cu}_{1-x}\text{O}$ is stable in the dark but corrodes to Cu_2O under illumination. (e) Cu- $L_{2,3}$ edges of CuO and Cu_2O distinguish between both copper oxidation states. The photocorrosion could be localized in a TEM cross section image (f and g) with corresponding EELS map (h), showing cubic Cu_2O crystals on the $\text{Li}_x\text{Cu}_{1-x}\text{O}$ surface. (i) Overview image of one crystal removed from a $\text{Li}_x\text{Cu}_{1-x}\text{O}$ film after an electrochemistry experiment performed for 15 min at 0.2 V under illumination, showing a roundish crystal overgrown by square crystals. (j) Average background subtraction filtered (ABSF) high resolution TEM image showing one square crystal at the surface of a spherical one. The FFTs of the marked regions were indexed for Cu_2O (k) and CuO (l), respectively.



mapping. Cu_2O grows as distinct crystallites on the surface of $\text{Li}_x\text{Cu}_{1-x}\text{O}$ instead of forming a dense layer. Additionally, there is no obvious Cu_2O gradient inside the films, as Cu_2O seems to form on all $\text{Li}_x\text{Cu}_{1-x}\text{O}$ nanocrystals exposed to water. The application of a thin $\text{Ti}_{0.8}\text{Nb}_{0.2}\text{O}_x$ coating by atomic layer deposition and the deposition of a platinum co-catalyst increased the stability of $\text{Li}_x\text{Cu}_{1-x}\text{O}$ against decomposition under hydrogen evolution.

■ **J. Kampmann, S. Betzler, H. Hajiyani, S. Häringer, M. Beetz, T. Harzer, J. Kraus, B. V. Lotsch, C. Scheu, R. Pentcheva, D. Fattakhova-Rohlfing, T. Bein:** *How photocorrosion can trick you: a detailed study on low-bandgap Li doped CuO photocathodes for solar hydrogen production;* *Nanoscale* 12, 7766 (2020).

3

CELLULOSE NANOCRYSTAL-TEMPLATED TIN DIOXIDE THIN FILMS FOR GAS SENSING

Alesja Ivanova, Bruno Frka-Petesic, Andrej Paul, Thorsten Wagner, Askhat N. Jumabekov, Yuri Vilks, Johannes Weber, Jörn Schmedt auf der Günne, Silvia Vignolini, Michael Tiemann, Dina Fattakhova-Rohlfing, and Thomas Bein

■ <https://bein.cup.uni-muenchen.de/>

■ https://www.fz-juelich.de/iek/iek-1/EN/Research/Department_ElectrochemicalStorage

Porous tin dioxide is an important low-cost semiconductor applied in electronics, gas sensors, and biosensors. In this collaborative project, the authors present a versatile template-assisted synthesis of nanostructured tin dioxide thin films using cellulose nanocrystals (CNCs). They demonstrate that the structural features of CNC-templated tin dioxide films strongly depend on the precursor composition. The precursor properties were studied by using low-temperature nuclear magnetic resonance spectroscopy of tin tetrachloride in solution. This way it was possible to optimize the precursor conditions to obtain homogeneous precursor mixtures and therefore highly porous thin

films with pore dimensions in the range of 10-20 nm. Moreover, by exploiting the high surface area of the material, the group developed a resistive gas sensor based on CNC-templated tin dioxide. The sensor shows high sensitivity to carbon monoxide (CO) in ppm concentrations and low cross-sensitivity to humidity. Most importantly, the sensing kinetics are remarkably fast; both the response to the analyte gas and the signal decay after gas exposure occur within a few seconds, faster than in standard SnO_2 -based CO sensors. This is attributed to the high gas accessibility of the very thin porous film.

■ **A. Ivanova, B. Frka-Petesic, A. Paul, T. Wagner, A. N. Jumabekov, Y. Vilks, J. Weber, J. Schmedt auf der Günne, S. Vignolini, M. Tiemann, D. Fattakhova-Rohlfing, T. Bein:** *Cellulose Nanocrystal-Templated Tin Dioxide Thin Films for Gas Sensing;* *ACS Applied Materials & Interfaces* 12, 12639 (2020).

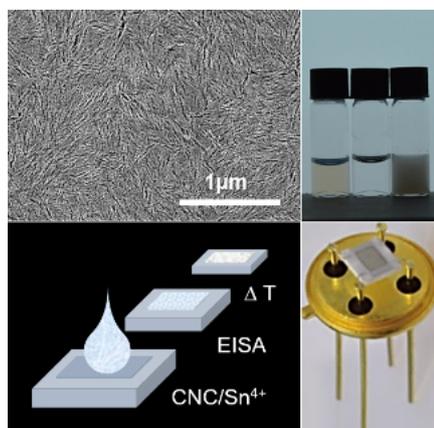


Fig. 1. Top left: SEM top-view image of tin oxide thin film prepared from 0.2 M tin chloride in 2 wt% aqueous suspension of cellulose nanocrystals. The suspensions were coated on silicon wafers and calcined at 400 °C. Top right: photographs of 2 wt% CNC suspension, 0.2 M SnCl_4 , and mixture of 2 wt% CNC and 0.2 M SnCl_4 in water (from left to right). Bottom left: schematic of the fabrication procedure for the CNC-templated porous tin dioxide sensor. Bottom right: photograph of the sensor substrate.

V(III)-DOPED NICKEL OXIDE-BASED NANOCATALYSTS FOR ELECTROCHEMICAL WATER SPLITTING: INFLUENCE OF PHASE, COMPOSITION, AND DOPING ON THE ELECTROCATALYTIC ACTIVITY

Daniel Böhm, Michael Beetz, Christopher Kutz, Siyuan Y. Zhang, Christina Scheu, Thomas Bein, and Dina Fattakhova-Rohlfing

Doped nickel oxide-based compounds are attracting great interest as very efficient and abundant catalysts and were thoroughly investigated as battery materials in the past. However, there is still no clear understanding of the influence of dopants on the complex dynamic character of their chemically and potential-driven transformations. In this collaboration, the group has developed a synthesis procedure enabling the controlled formation of nanosized nickel hydroxide and nickel oxide polymorphs substituted with vanadium(III) [V(III)] ions and further investigated their structure-activity correlation for electrochemical water oxidation. This work therefore primarily focuses on an in-depth structural characterization of the homogeneously doped nanosized alpha- and beta-Ni(OH)₂ polymorphs. It could be shown that concentrations of 10 at. % V(III) and higher can effectively inhibit a spontaneous phase

transformation known as chemical aging of the turbostratic alpha-phase to the more crystalline beta-Ni(OH)₂ phase in neutral aqueous media. The Fe-impurity-based electrocatalytic activity determined for alpha-/beta-Ni_{1-x}V_x(OH)₂ showed only a minor increase of 10% oxygen evolution reaction (OER) activity for a 1 at. % doped nonaged sample resembling the alpha-phase, while a 5 at. % V(III)-doped sample chemically aged over 24 h led to a doubled OER activity versus the undoped reference, which transformed into beta-Ni(OH)₂ over that period of time.

■ D. Böhm, M. Beetz, C. Kutz, S. Y. Zhang, C. Scheu, T. Bein, and D. Fattakhova-Rohlfing: *V(III)-Doped Nickel Oxide-Based Nanocatalysts for Electrochemical Water Splitting: Influence of Phase, Composition, and Doping on the Electrocatalytic Activity*, *Chemistry of Materials* 2020, 32, 10394.

INCREASING THE STABILITY OF DNA NANOSTRUCTURES AND FLUORESCENT LABELS FOR SINGLE-MOLECULE AND SUPER-RESOLUTION MICROSCOPY

Lennart Grabenhorst, Michael Scheckenbach, Tom Schubert, Carsten Forthmann, Kateryna Trofymchuk, Florian Steiner, Viktorija Glembockytė, and Philip Tinnefeld

■ <https://tinnfeld.cup.uni-muenchen.de>

DNA nanotechnology and advances in the DNA origami technique have enabled facile design and synthesis of complex and functional nanostructures creating emerging potentials for e.g. drug delivery, nanophotonics and biosensing. Molecular devices are, however, prone to rapid degradation due to the

high proportion of surface atoms on the nanoscale and due to their complex and demanding working environments.

Understanding the degradation pathways of molecular devices is a crucial step towards the design of robust and functional nanostructures. Fluorescent

dyes are often a bottleneck for such devices because of their irreversible photobleaching. Due to the up-concentration of light in a plasmonic hotspot, conditions for fluorescent dyes are even more demanding in DNA origami nanoantennas. Despite the improved photostability of a single fluorophore by these nanoantennas, its performance in the hotspot is limited by photophysical processes, such as formation of dim states and photoisomerization. These processes limit the photon count rates, increase heterogeneity, complicate quantification of fluorescence enhancement and reduce the achievable time resolution in biophysical single-molecule experiments. For instance, the photophysics of a DNA hairpin assay with a fluorophore-quencher pair is heavily influenced by plasmonic effects, resulting in false positives due to premature photobleaching of the quencher.

To overcome the fast device degradation on the nanoscale, approaches for the self-repair of functional molecular devices are desirable. Inspired by nature's self-repair mechanisms at the molecular level, the self-assembly and reconfigurability of DNA origami nanostructures can be exploited to induce the dynamic self-repair of photoinduced and enzymatic defects. By dynamically exchanging

building units with intact analogues from solution, the function of a brightness reference structure can be recovered even after complete photodamage and the integrity of super-resolution nanorulers used for DNA PAINT can be maintained over days even in degrading conditions as serum. Based on the given examples, the two possible self-repair mechanisms using this approach are illustrated: the damage unspecific self-regeneration, which exchanges intact and defective building units, and the damage specific self-healing, i.e. the exchange of only defective building units.

■ **L. Grabenhorst, K. Trofymchuk, F. Steiner, V. Glembockyte, P. Tinnefeld:** *Fluorophore Photostability and Saturation in the Hotspot of DNA Origami Nanoantennas*, *Methods Appl. Fluoresc.* 8, 024003, DOI 10.1088/2050-6120/ab6ac8 (2020)

■ **M. Scheckenbach, T. Schubert, C. Forthmann, V. Glembockyte, P. Tinnefeld:** *Self-Regeneration and Self-Healing in DNA Origami Nanostructures*, *Angew. Chem. Int. Ed.*, DOI 10.1002/anie.202012986 (2020)



Fig. 1 Artificial DNA nanoruler that autonomously repairs defects via incorporation of new building blocks (Image: Vera Hiendl, e-conversion).

HOW TO CLAMP GENES

Kevin Kramm, Tim Schröder, Jerome Gouge, Andrés Manuel Vera, Kapil Gupta, Florian B. Heiss, Tim Liedl, Christoph Engel, Imre Berger, Alessandro Vannini, Philip Tinnefeld, and Dina Grohmann

■ <https://tinnefeld.cup.uni-muenchen.de/>

■ https://www.softmatter.physik.uni-muenchen.de/liedl_group/index.html

Transcription of the genomic DNA into RNA is a necessary process in every cell that provides the blueprints and building materials for protein synthesis. The transcription is regulated by transcription factors which guide the RNA polymerase to the genes. An interdisciplinary team consisting of physicist Prof. Tim Liedl, physicochemist Prof. Philip Tinnefeld and biochemist Prof. Dina Grohmann from the University of Regensburg tackled the question how transcription factors react to tiny forces. The researchers used the DNA origami force clamp structure (P. Nickels et al., *Science*, 2016) to mimic the forces exerted on the DNA by cellular processes in the nucleus between 0 and 15 pico-Newton. Binding of the eukaryotic transcription factor TATA-binding protein to its TATA-box recognition sequence leads to a bending of the ds-DNA which was detected with two fluorescence dyes by Förster resonance energy transfer due to a change in inter dye distance. Single-molecule studies finally resolved changes in the binding population for different forces and different transcription factors. The team demonstrated that the specialized RNA polymerase III requires the additional factor Bdp1 that interconnects all components of the multimeric transcription initiation factor complex. This stably bound platform can recruit RNA polymerase III for multiple rounds of transcription, ensuring a high output of tRNAs that are critical for cell growth and proliferation.

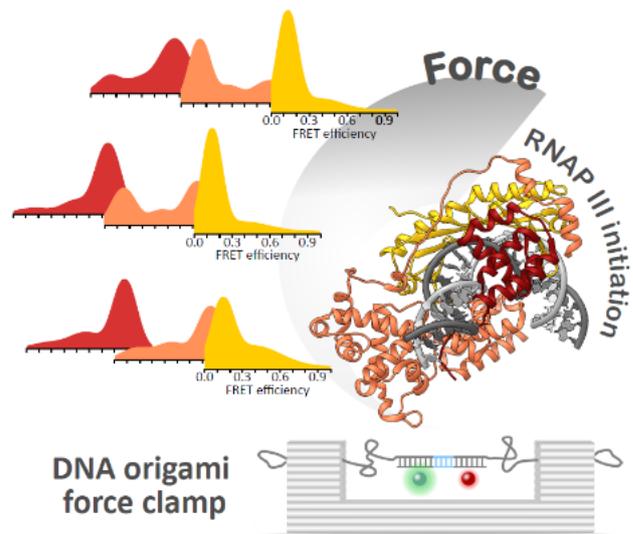


Fig. 1. Top left: Change in FRET populations for different forces for different transcription factors. **Right:** Sketch of the RNA polymerase initiation complex with Bdp1.

Bottom: Sketch of the DNA origami force clamp with the FRET-pair highlighted as green and red dot.

■ K. Kramm, T. Schröder, J. Gouge, A.M. Vera, K. Gupta, F.B. Heiss, T. Liedl, C. Engel, I. Berger, A. Vannini, P. Tinnefeld, D. Grohmann: *DNA origami-based single-molecule force spectroscopy elucidates RNA Polymerase III pre-initiation complex stability*; *Nat. Commun.* 11(2828), DOI: 10.1038/s41467-020-16702-x (2020).

PULSED INTERLEAVED MINFLUX

Luciano A. Masullo, Florian Steiner, Jonas Zähringer, Lucia F. Lopez, Johann Bohlen, Lars Richter, Fiona Cole, Philip Tinnefeld, and Fernando D. Stefani

■ <https://tinnfeld.cup.uni-muenchen.de>

Super-resolution microscopy techniques like STED and STORM/PALM have revolutionized the use of optical microscopes to study biological systems at dimensions well below the diffraction limit. The latest development in super-resolution is MINFLUX. It combines the stochastic and deterministic nature of the basic techniques and achieves a molecular-scale resolution of ~ 1 nm.

The groups of Prof. Philip Tinnefeld and Prof. Fernando Stefani from the University of Buenos Aires (Argentina) developed p-MINFLUX, a new implementation of the highly photon-efficient single-molecule localization method with a simplified experimental setup and additional fluorescence lifetime information. In contrast to the original MINFLUX implementation, p-MINFLUX uses interleaved laser pulses to deliver the doughnut-shaped excita-

tion foci at a maximum repetition rate. Using both static and dynamic DNA origami model systems, the groups demonstrated the performance of p-MINFLUX for single-molecule localization nanoscopy and tracking, respectively. p-MINFLUX delivers 1–2 nm localization precision with 2000 – 1000 photon counts. In addition, p-MINFLUX gives access to the fluorescence lifetime enabling future applications for multiplexing and super-resolved lifetime imaging. p-MINFLUX should help to unlock the full potential of innovative single-molecule localization schemes.

■ **L. A. Masullo, F. Steiner, J. Zähringer, L. F. Lopez, J. Bohlen, L. Richter, F. Cole, P. Tinnefeld, F. D. Stefani:** *Pulsed Interleaved MINFLUX*; Nano Letters, DOI: 10.1021/acs.nanolett.0c04600 (2021).

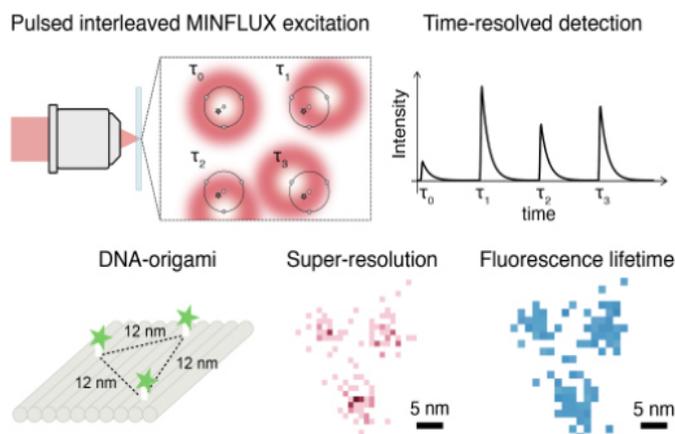


Fig. 1. Top row: Principle of p-MINFLUX: spatial (left) and temporal (right) distribution of the excitation laser pulses; **bottom row:** super-resolution (center) and fluorescence lifetime (right) image of a static DNA origami labelled with three dyes at a distance of ~ 12 nm (left).

THERMAL HABITAT FOR RNA AMPLIFICATION AND ACCUMULATION

Annalena Salditt, Lorenz M. R. Keil, David P. Horning, Christof B. Mast, Gerald F. Joyce, and Dieter Braun

■ <https://www.biosystems.physik.uni-muenchen.de>

We could finish a very fruitful collaboration in the Simons collaboration on the Origins of life, between the Braun lab and Jerry Joyce at Salk Institute, leading to a publication in Physical Review Letters (doi.org/10.1103/PhysRevLett.125.048104). The finding also triggered an overview article in the APS journal physics: physics.aps.org/articles/v13/117. In this work, we could show that not only that Ribozymes, the major molecules of the RNA world hypothesis could be thermally cycled simply by a millimeter-sized convection in a simulated rock pore, yielding very similar if not better replication yields as compared to the thermal cycler where these reactions were run before (doi.org/10.1073/pnas.1610103113). But our finding also set the stage on what is necessary to combine the replication driven by a Ribozyme with the thermal accumulation of the RNA itself. We did already now see accumulation of RNA and the Ribozyme to replicate the RNA in colder areas of the convection. This “rescue into the cold” significantly increased

the lifetime of the Ribozyme in the convection setting. Interestingly this was because we observed that the Ribozyme was aggregating already under its working conditions, a fact that was not determined before. But what was perhaps most crucial is that we could simulate the system fully on a computer, a step that will allow us to first explore conditions of replication and accumulation in the future by finite element analysis. With both this simulation capability and further progress in the selection of Ribozymes, we are likely to be able to tune the system such that it is pushed by the physical length selection that it can actually replicate longer sequences than the 35mer selected by the two primers in this experiment. So we are not too far away from replicating autonomously RNA information and start Darwinian evolution. We are evaluating different settings in the computer to add a robust length selection and look forward to the next iteration of this collaboration.

■ **A. Salditt, L. M. R. Keil, D. P. Horning, C B. Mast, G. F. Joyce, and D. Braun:** *Thermal Habitat for RNA Amplification and Accumulation*; Physical Review Letters [doi:https://doi.org/10.1103/PhysRevLett.125.048104](https://doi.org/10.1103/PhysRevLett.125.048104) (2020).

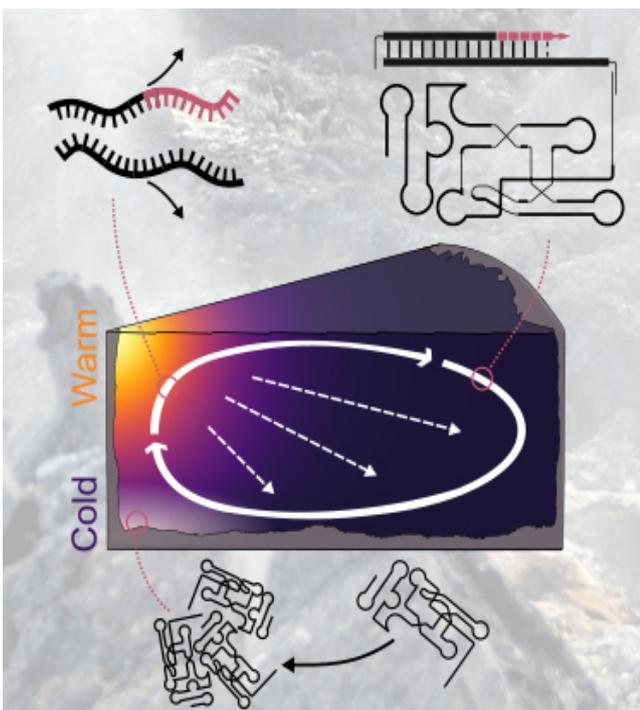


Fig. 1. RNA can be replicated by RNA in a temperature hot spot. The interesting feature is that the RNA molecules accumulate towards at the colder area where they survive orders of magnitude longer. The combination is a possible setting to start molecular evolution with RNA only.

CHIRAL ASSEMBLY OF GOLD/SILVER CORE SHELL PLASMONIC NANORODS ON DNA ORIGAMI WITH STRONG OPTICAL PROPERTIES

Linh Nguyen, Mihir Dass, Martina Ober, Lucas Besteiro, Zhiming Wang, Bert Nickel, Alexander Govorov, Tim Liedl, and Amelie Heuer-Jungemann

■ <https://www.biochem.mpg.de/de/heuer-jungemann>

■ https://www.softmatter.physik.uni-muenchen.de/liedl_group

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

This research project was a fruitful collaboration between the Liedl/Heuer-Jungemann and Nickel groups. In this work we presented a method for synthesizing highly stable gold-silver core-shell NRs that are instantaneously functionalized with DNA, enabling chiral self-assembly on DNA origami. The thickness of the silver shell as well as conformation of the conjugated DNA were analyzed in detail by Small and Wide-Angle X-Ray Scattering (SAXS and WAXS), which gave detailed insights into the nature of the shells not attainable through visual means. The silver shell gives rise to an enhancement of plasmonic properties, reflected here in strongly increased circular dichroism, as compared to pristine gold nanorods. Gold-silver nanorods are ideal candidates for plasmonic sensing with increased sensitivity as needed in pathogen RNA or antibody testing for nonlinear optics and light-funneling applications in surface enhanced Raman spectroscopy. Furthermore, the control of interparticle orientation enables the study of plasmonic phenomena, in particular, synergistic effects arising from plasmonic coupling of such bimetallic systems. Currently, these nanorods are being investigated for use in lateral flow assays and a spin-off company will be formed.

■ L. Nguyen, M. Dass, M. Ober, L.V. Besteiro, Z. M. Wang, B. Nickel, A.O. Govorov, T. Liedl, A. Heuer-Jungemann: *Chiral Assembly of Gold/Silver Core Shell Plasmonic Nanorods on DNA Origami with Strong Optical Properties*; ACS Nano, doi: 10.1021/acsnano.0c03127 (2020).

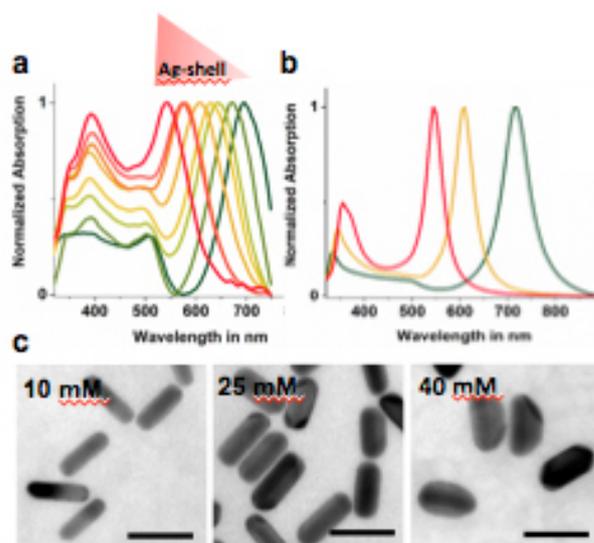


Fig. 1. (a) Absorption spectra of Au/AgNRs@DNA synthesized with varying AgNO_3 concentrations (10 – 40 mM). (b) Simulated extinction spectra of Au/AgNRs. (c) TEM images of Au/AgNRs@DNA). Scale bars are 40 nm.

SYNTHESIS AND LARGE-SCALE ASSEMBLY OF HYBRID COLLOIDS FOR APPLICATIONS IN SENSING, PHOTOCATALYSIS AND ELECTROCATALYSIS

Seunghoon Lee, Joong Bum Lee, Harriet Walker, Stefan Maier, and Emiliano Cortés

■ <https://www.hybridplasmonics.org>

Photons, electrons, and phonons can be channeled and manipulated to create plasmonic and photonic chemical hotspots [1]. Plasmons for example, have opened access to enhance and control chemical reactivity and selectivity with CW illumination in the visible range, a fundamental requisite for sunlight photocatalysis [1,4]. Further understanding and control of these processes could influence potential industrial applications of photocatalysis, which so far have remained elusive. In this sense, we have recently reported a novel synthesis route towards efficient hybrid plasmonic catalysts, as shown in the left side of the Figure for bimetallic trimers. These structures can highly enhance light absorption and energy transfer to molecular species compared to their monometallic and/or monomeric counterparts [3]. Another bottleneck for large-scale applications of colloidal nanomaterials in sensing or catalysis is their deterministic positioning and assembly onto substrates (electrodes, supports, etc.) [5]. This is a core requirement and a promising alternative to top-down lithography to create functional nanostructures and nanodevices. To address this problem, we have developed a template dissolution interfacial patterning (TDIP) technique to assemble and print single colloidal AuNP arrays onto various dielectric and conductive substrates in the absence of any adhesion layer, with printing yields higher than 98% and covering areas of $\sim\text{cm}^2$. The TDIP approach – shown in the right side of the Figure – grants direct access to the interface between the AuNP and the target surface, enabling the use of

colloidal AuNPs as building blocks for practical applications such as electro- and photoelectrochemistry and sensing [2].

■ **E. Cortés, L.V. Besteiro, A. Alabastri, A. Baldi, G. Tagliabue, A. Demetriadou, Prineha Narang:** *Challenges in Plasmonic Catalysis*; ACS Nano 14 (12), 16202–16219 (2020).

■ **J. B. Lee, H. Walker, Y. Li, T. W. Nam, A. Rakovich, R. Sapienza, Y. S. Jung, Y. S. Nam, S. A. Maier, E. Cortés:** *Template Dissolution Interfacial Patterning of Single Colloids for Nanoelectrochemistry and Nanosensing*; ACS Nano 14 (12), 17693–17703 (2020).

■ **S. Lee, H. Hwang, W. Lee, D. Schebarchov, Y. Wy, J. Grand, B. Auguie, D. H. Wi, E. Cortés, S. W. Han:** *Core–Shell Bimetallic Nanoparticle Trimers for Efficient Light-to-Chemical Energy Conversion*; ACS Energy Letters 5 (12), 3881–3890 (2020).

■ **E. Cortés, A. O. Govorov, H. Misawa, K. A. Willets:** *Special topic on emerging directions in plasmonics*; J. Chem. Phys., 153 (1), 010401 (2020).

■ **S. Bell, G. Charron, E. Cortés, J. Kneipp, M. Lamy de la Chapelle, J. Langer, M. Procházka, V. Tran, S. Schlücker:** *Towards Reliable and Quantitative SERS: from Key Parameters to Good Analytical Practice*; Angewandte Chemie International Edition, 59, 5454 – 546 (2020).

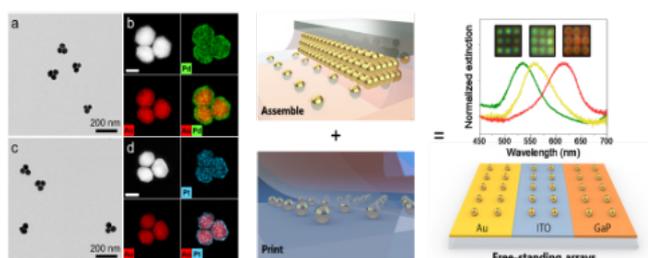


Fig. 1: TEM images of the colloidal bimetallic trimers for plasmonic catalysis. In **a)** and **b)** Au@Pd nanoparticles were synthesized and in **c)** and **d)** Au@Pt trimers were prepared. In the right side of the figure we show an scheme of the new “template dissolution” soft-lithography method to pattern large-scale arrays of colloidal nanoparticles.

METAL-ORGANIC FRAMEWORK NANOPARTICLES INDUCE PYROPTOSIS IN CELLS

Evelyn Plötz, Andreas Zimpel, Valentina Cauda, David Bauer, Don C. Lamb, Christoph Haisch, Stefan Zahler, Angelika Vollmar, Stefan Wuttke, and Hanna Engelke

■ <http://wuttkescience.com>

■ <https://pharmazie.uni-graz.at/de/forschen-alt/pharmazeutische-chemie>

■ <https://www.cup.uni-muenchen.de/pc/lamb>

In previous collaborations, we could show that metal-organic framework nanoparticles can serve as platform for the delivery of drugs. For such biomedical applications, the nanoparticles are inert carriers that transport active drugs to the target tissue and thus impact pharmacokinetics. However, they also have the potential to act as active drug themselves and influence the pharmacodynamics. Specifically, nanoparticles build from ions show great potential in this respect. Most ions are fairly harmless, since their intracellular concentrations are strictly regulated by cells. However, if large ion concentrations are released into the cytosol, programmed cell death is induced. In this publication, we use Fe-based MOF-nanoparticles (MIL-100(Fe)) as combined drug and carrier in one to release toxic concentrations of iron ions into cells. A lipid coating around the nanoparticles facilitates stealth iron import into the cells, where the nanoparticles degrade and release iron ions into the cytosol. Subsequently, cells undergo pyroptosis – a cell death involving the immune response.

Remaining iron-ions will again be subject to the cellular regulation, and harmless to neighboring cells. Hence, the lipid-coated nanoparticles turn largely un toxic iron ions into a toxic drug by virtue of their nanoarchitecture and their coating. The degradation of the nanoparticles, and thus their toxicity, is limited to slightly acidic extracellular pH. This allows for selectivity – a key property for therapeutics. Based on these properties, the nanoparticles may be used in the future as therapeutics against tumors, which grow in acidic microenvironments. The particles may reduce the tumor and the induced pyroptosis may at the same time stimulate an anti-tumor immune response.

■ **E. Plötz, A. Zimpel, V. Cauda, D. Bauer, D. Lamb, C. Haisch, S. Zahler, A. Vollmar, S. Wuttke, H. Engelke:** *Metal-Organic Framework Nanoparticles Induce Pyroptosis in Cells Controlled by the Extracellular pH*; *Adv. Mater.*, doi: 10.1002/adma.201907267 (2020).

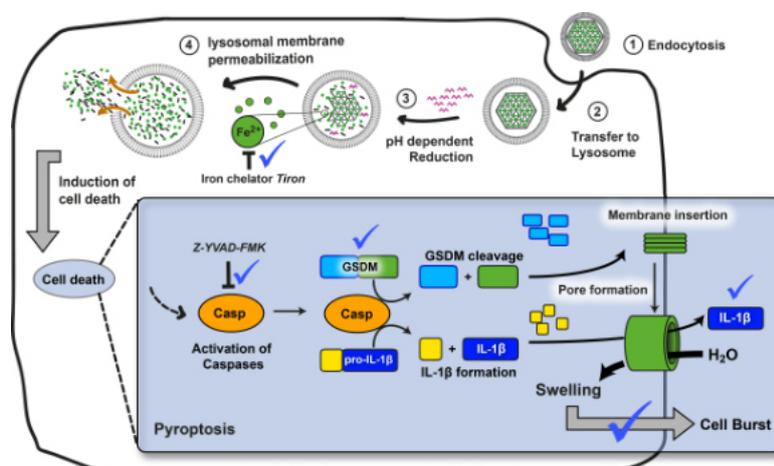


Fig. 1. Lipid-coated metal-organic framework nanoparticles MIL-100(Fe) are taken up by cells. In the cell, they are degraded, released into the cytosol and induce pyroptosis, a programmed cell death involving the immune system.

DESIGNING MOLECULES ON A FORCE SENSOR TO PRECISELY INVESTIGATE THE FUNCTION OF BIO-MOLECULES

Leonard C. Schendel, Magnus S. Bauer, Steffen M. Sedlak, Carleen Kluger, Diana A. Pippig, Lukas F. Milles, Martin Benoit, Jan Lipfert, and Hermann E. Gaub

■ <https://www.biophysik.physik.uni-muenchen.de>

■ <https://www.molecularbiophysics.physik.uni-muenchen.de>

The binding complex of the small molecule biotin and the homotetrameric protein streptavidin (SA) is essential for fundamental assays and applications in biosciences. Therefore, the behavior of this extraordinarily high-affinity interaction under mechanical force is studied intensively not only by applying single-molecule force spectroscopy (SMFS). Several all-atom steered molecular dynamics (SMD) simulations for the entire system, have identified different force pathways for the dissociation of biotin from SA [1].

Involving these findings by genetically modifying the SA tetramer, the interaction force with biotin not only was optimized, but also became tunable by external conditions (Figure 1) [2].

Complementing the AFM characterizations of this interaction, the properties of the individual SA monomers also were scrutinized by magnetic tweezers (MT) in a collaboration with Jan Lipfert. Utilizing the high precision of the AFM force experiments pulling an individual biotin from a SA-binding-pocket immobilized in a zero mode wave guide, allowed to characterize the diffusion times of fluorescently labelled biotin replacing the removed biotin by single molecule fluorescence [3].

Also for highly complex molecular arrangements as found in cells such force experiments can be successfully applied [4] demasking an AFM force sensor as "lab on a tip" [5].

Finally the explanation of the discrepancy between the strongest non-covalent force and its rather fast dissociation in the absence of force -recently discovered between the prototypical staphylococcal adhesin SdrG targeting the short peptide from human fibrinogen β - has been elucidated [6].

■ [1] Steffen M. Sedlak, Leonard C. Schendel, Hermann E. Gaub and Rafael C. Bernardi: *Streptavidin/biotin: Tethering geometry defines unbinding mechanics*; Science Advances, DOI: 10.1126/sciadv.aay5999 (2020).

■ [2] Leonard C. Schendel, Steffen M. Sedlak and Hermann E. Gaub: *Switchable reinforced streptavidin*; Nanoscale, DOI: 10.1039/d0nr00265h (2020).

■ [3] Leonard C. Schendel, Magnus S. Bauer, Steffen M. Sedlak, Hermann E. Gaub: *Single-Molecule Manipulation in Zero-Mode Waveguides*; Small Journal, DOI: 10.1002/sml.201906740 (2020).

■ [4] Carleen Kluger, Lukas Braun, Steffen M. Sedlak, Diana A. Pippig, Magnus S. Bauer, Ken Miller, Lukas F. Milles, Hermann E. Gaub, Viola Vogel: *Different Vinculin Binding Sites Use the Same Mechanism to Regulate Directional Force Transduction*; Biophysical Journal, doi.org/10.1016/j.bpj.2019.12.042 (2020).

■ [5] D. J. Müller, A. C. Dumitru, C. Lo Giudice, Hermann E. Gaub, P. Hinterdorfer, G. Hummer, J.J. De Yoreo, Y.F. Dufrene, D. Alsteens: *Atomic Force Microscopy-Based Force Spectroscopy and Multiparametric Imaging of Biomolecular and Cellular Systems*; Chem Rev., doi: 10.1021/acs.chemrev.0c00617 (2020).

■ [6] Lukas F. Milles and Hermann E. Gaub: *Extreme mechanical stability in protein complexes*; Curr. Op. in Struct. Biol., doi.org/10.1016/j.sbi.2019.11.012 (2020).

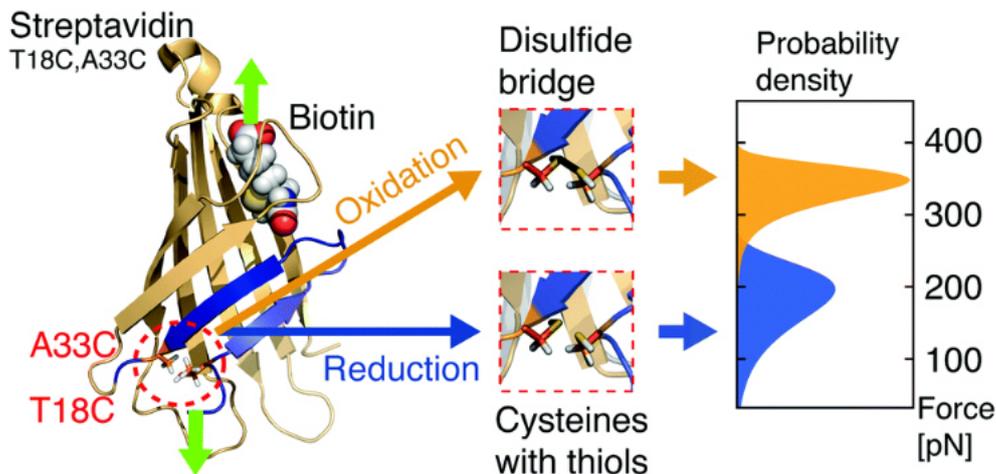


Fig. 1. Switchable reinforced streptavidin. We introduced two mutations (T18C,A33C) in the functional subunit of monovalent streptavidin to establish a switchable connection (disulfide bridge) between the first two β -strands to prevent a destabilizing unfolding. In AFM based SMFS experiments, we observed unbinding forces of about 350 pN (at 10 nN/s) for pulling a single biotin out of an N-terminally anchored monovalent SA binding pocket – about 1.5-fold higher compared with what has been reported for N-terminal force loading of native monovalent SA. Upon addition of a reducing agent, the unbinding forces dropped back to 200 pN, as the disulfide bridge was destroyed. Switching from reducing to oxidizing buffer conditions, the inverse effect was observed. This illustrates how the mechanics of a receptor–ligand system can be tuned by engineering the receptor protein far off the ligand-binding pocket.

13

ELECTRONIC TEMPERATURE DEPENDENT SUPPRESSION OF INTERFERING QUANTUM PATHWAYS IN GRAPHENE RAMAN SCATTERING

Veit Giegold, Lucas Lange, Richard Ciesielski, and Achim Hartschuh

<https://physchem.cup.uni-muenchen.de/hartschuh/>

Raman spectroscopy is a key tool for the investigation of graphene and other sp^2 carbon allotropes. Graphene’s characteristic Raman signals give access to particular rich physics, because of its intricate electron–phonon coupling and strong electronic resonances, which are the origin of its facile detection. The Raman spectrum of pristine graphene is dominated by two characteristic bands: The G and the 2D band that can be assigned to single and double resonant processes involving different numbers of intermediate states. The spectral shape and amplitude of the 2D band sensitively depends on the electronic coupling between the

sheets in few layer graphene, such that the symmetry of the 2D band and the intensity ratio 2D/G can be utilized as the key characteristics to determine the layer number.

We show that the Raman scattering signals of the two dominant Raman bands G and 2D of graphene sensitively depend on the laser intensity in opposite ways. High non-equilibrium electronic temperatures reached for pulsed laser excitation lead to an asymmetric Fermi–Dirac distribution at the different optically resonant states contributing to Raman scattering. This results in a partial Pauli blocking of destructively interfering quantum pathways for G

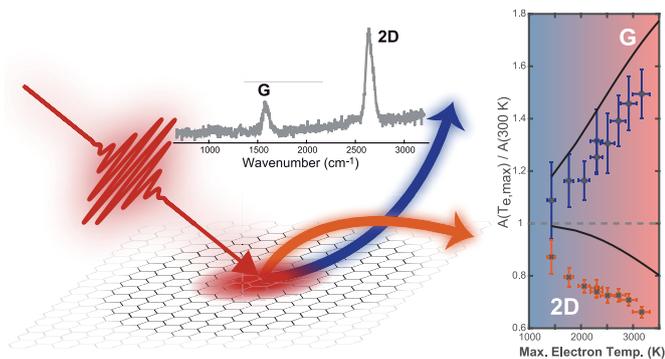


Fig. 1. The Raman G and 2D band intensities in graphene result from electronic-temperature dependent interference of quantum pathways.

band scattering, which is observed as a super-linear increase of the G band intensity with laser power. The 2D band, on the other hand, exhibits sub-linear

intensity scaling due to the blocking of constructively interfering contributions.

The opposite intensity dependencies of the two bands are found to reduce the observed 2D/G ratio by more than factor two, which has to be taken into account while deriving layer numbers. Because electronic temperatures can vary far more rapidly than that of phonon populations due to highly efficient electron–electron scattering, this effect is also expected to influence the signal dynamics observed in time-resolved studies of the Raman scattering intensities of graphene.

■ **V. Giegold, L. Lange, R. Ciesielski, A. Hartschuh:** *Non-linear Raman scattering intensities in graphene*; *Nanoscale*, DOI: 10.1039/c9nr10654e (2020).

14

CONDENSATION SIGNATURES OF PHOTOGENERATED INTERLAYER EXCITONS IN 2D HETEROSTACKS

Alexander Holleitner

■ <https://www.wsi.tum.de/views/groups.php?group=holleitner>

Increasing the interaction strength between quasiparticles in solid-state materials can cause strong correlations, collective phenomena and the transition to large-scale quantum phases, for example to a Bose-Einstein condensate. Heterostructures made of semiconducting 2D materials, such as MoSe₂ and WSe₂, are ideal systems to realize a condensation of excitons. The latter are Coulomb-bound electron hole pairs. The heterostructures enable large exciton binding energies, long photoluminescence lifetimes, as well as a permanent exciton dipole, which allows the manipulation of the exciton ensembles, e.g. via electric fields. The Holleitner group observed several signatures regarding photoluminescence intensity, linewidth, temporal coherence and excitonic propagation dynamics in accordance with the predicted condensation temperature of an excitonic Bose-Einstein condensation at about 10 Kelvin. This results opens the avenue to investigate quantum

mechanical many-body physics of excitons in nanostructured circuits.

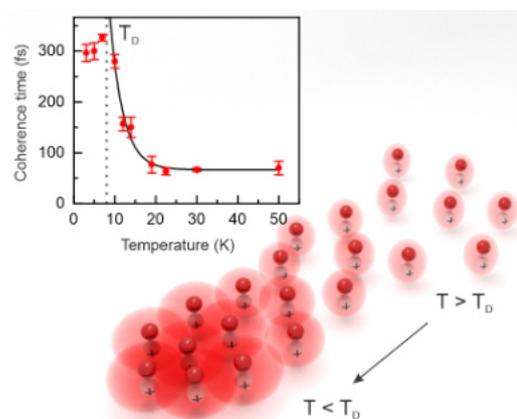


Fig. 1. Below a degeneracy temperature T_D , a many-body state emanates of interacting excitons, giving rise to an enhanced coherence time and excellent optical properties of the exciton ensemble.

■ L. Sigl, F. Sigger, F. Kronowetter, J. Kiemle, J. Klein, K. Watanabe, T. Taniguchi, J. J. Finley, U. Wurstbauer, A. W. Holleitner: *Condensation signatures of photogenerated interlayer excitons in a van der Waals heterostack*, Physical Review Research 2, 042044(R) (2020).

■ J. Kiemle, F. Sigger, M. Lorke, B. Miller, K. Watanabe, T. Taniguchi, A. W. Holleitner, U. Wurstbauer: *Control of the orbital character of indirect excitons in MoS₂/WS₂ heterobilayers*, Phys Rev B 101, 121404 (R) (2020).

15

ATOMISTIC POSITIONING OF SINGLE QUANTUM EMITTERS IN SEMICONDUCTING 2D MATERIALS

Alexander Holleitner

■ <https://www.wsi.tum.de/views/groups.php?group=holleitner>

Structuring materials with atomic precision is the ultimate goal of nanotechnology and is becoming increasingly relevant as an enabling technology for quantum electronics, spintronics, and optoelectronics, as well as for energy conversion applications. The Holleitner group demonstrated how to generate optically active defects in atomically thin 2D materials on a spatial scale of below 10 nm, such that scalable optoelectronics based on individual atomic states seems at reach. Until now, this goal was reserved only to materials and methods in the ultra-high vacuum. The Holleitner group uses a helium-ion microscope (HIM) to generate individual defects, e.g. in semiconducting MoS₂. The atomistic defects turn out to act as single photon emitters, which can be generated in large scale matrices with the mentioned accuracy. Moreover, the atomistic emitters can be integrated into field-effect

heterostacks allowing a gate-switching of the single photon emission.

■ E. Mitterreiter, et al.: *Atomistic Positioning of Defects in Helium Ion Treated Single-Layer MoS₂*, Nano Letters 20, 4437 (2020).

■ K. Barthelmi, et al.: *Atomistic defects as single-photon emitters in atomically thin MoS₂*, Applied Physics Letters Perspective 117, 070501 (2020).

■ J. Klein, L. Sigl, et al.: *Engineering the luminescence and generation of individual defect emitters in atomically thin MoS₂*, ACS Photonics 8, 2, 669 (2021).

■ A. Hötger, et al.: *Gate-switchable arrays of quantum light emitters in contacted monolayer MoS₂ van der Waals heterodevices*, Nano Letters 21, 1040

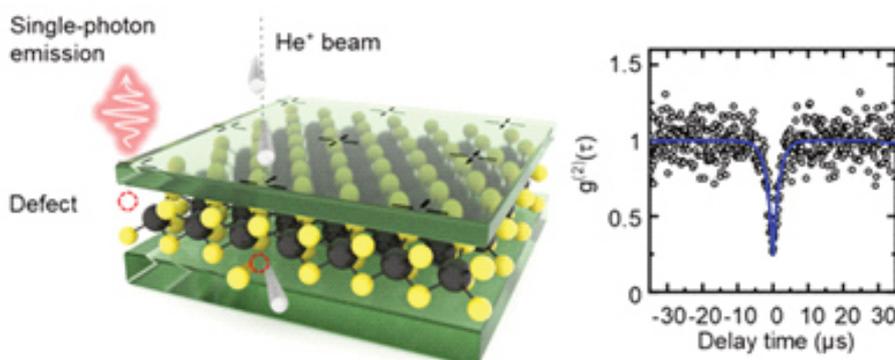


Fig. 1. Heterostack of a MoS₂ monolayer embedded with hBN with single sulphur vacancies induced by a focused helium-ion beam. The vacancies are positioned with an accuracy <10nm and act as single photon sources.

RATIONAL DESIGN OF COBALOXIME-COVALENT ORGANIC FRAMEWORK HYBRIDS FOR ENHANCED PHOTOCATALYTIC HYDROGEN EVOLUTION

Kerstin Gottschling, Gökçen Savasci, Hugo Vignolo-González, Sandra Schmidt, Philipp Mauker, Tanmay Banerjee, Petra Rovó, Christian Ochsenfeld, and Bettina V. Lotsch

■ <https://www.rovolab.org>

■ <https://www.fkf.mpg.de/lotsch>

■ <https://www.cup.uni-muenchen.de/pc/ochsenfeld>

Nature and its photosynthetic machinery have been an inspiration for synthetic chemists over the past decades. Covalent organic frameworks (COFs) – crystalline porous polymers entirely made from light elements – have become a unique platform to emulate and orchestrate artificial photocatalytic processes at the molecular level with high chemical and spatial precision. In this work, we have taken existing COF-based photocatalysts to the next level and developed an overall heterogeneous, all-single-site COF hybrid system based on a covalently bound co-catalyst, which improves the activity in comparison to physisorbed systems.

In this collaborative work between the groups of Petra Rovó, Christian Ochsenfeld and Bettina Lotsch, we successfully incorporated an azide-functionalized chloro(pyridine)cobaloxime moiety into a highly stable, hydrazine-based covalent organic framework backbone. This modification enhanced and prolonged the photocatalytic activity of cobaloxime in light-driven hydrogen evolution experiments compared to the un-bound system. The higher photocatalytic activity and improved long-term stability of the designed cobaloxime-tethered COF materials make them promising catalysts for future high-precision solar fuel technologies.

A challenging aspect of the work was to prove that anchoring by click reaction was successful and the functionalized COF contains covalently attached cobaloxime groups. Solid-state NMR in combination with quantum chemical calculations were crucial to prove that this is indeed what happened. Based on various structural models derived from molecular dynamics simulations, we calculated proton and

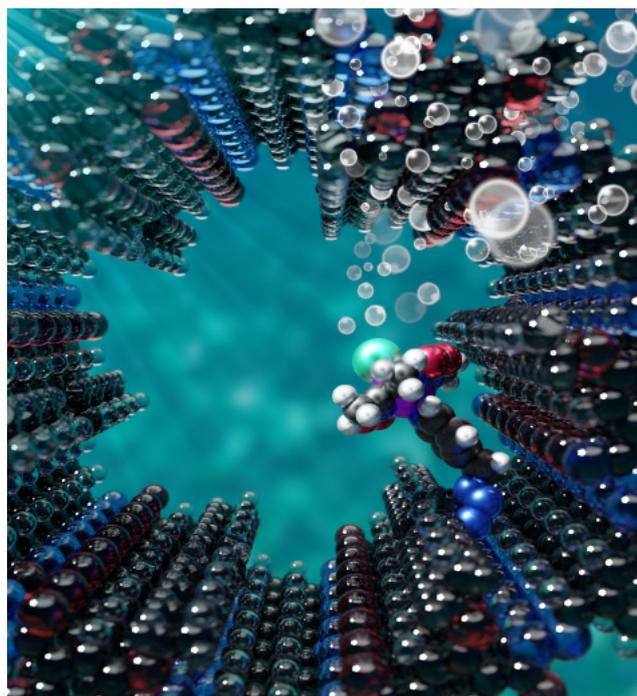


Fig. 1. An azide-functionalized chloro(pyridine)-cobaloxime immobilized on a hydrazine-based covalent organic framework backbone.

carbon chemical shifts at the quantum-chemical level, from which we constructed 1H - 1H and 1H - 13C 2D spectra for comparison to the experimental data. Such an approach allowed for the spectrum assignment and also enabled the detailed structural analysis of the system. We concluded that the significant improvements in photocatalytic activity could be a consequence of the close proximity between the cobaloxime unit and the COF pore wall. This finding puts the spotlight on confinement effects in porous photocatalytic systems and opens up new perspectives for rational catalyst design.

■ K. Gottschling, G. Savasci, H. Vignolo-González, S. Schmidt, P. Mauker, T. Banerjee, P. Rovó, C. Ochsenfeld, and B. V. Lotsch: *Rational Design of Covalent Cobaloxime–Covalent Organic Framework Hybrids for Enhanced Photocatalytic Hydrogen Evolution*; *J. Am. Chem. Soc.* 10.1021/jacs.0c02155 (2020).

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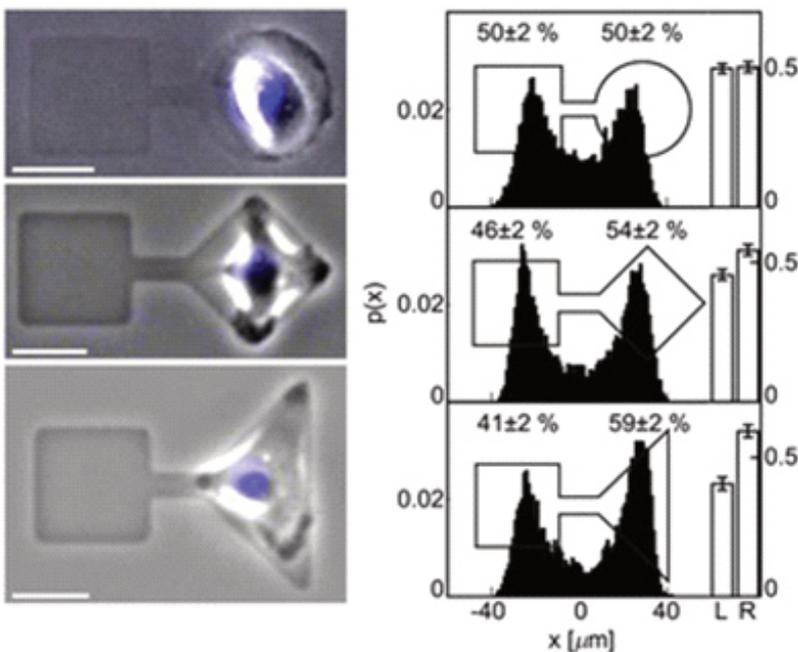
AREA AND GEOMETRY DEPENDENCE OF CELL MIGRATION IN ASYMMETRIC TWO-STATE MICROPATTERNS

Alexandra Fink, David B. Brückner, Christoph Schreiber, Peter J. F. Röttgermann, Chase P. Broedersz and Joachim O. Rädler

■ <https://www.softmatter.physik.uni-muenchen.de>
 ■ <https://research.vu.nl/en/persons/chase-broedersz>

Microstructured surfaces provide a unique framework to probe cell migration and cytoskeletal dynamics in controlled anchorage conditions. To investigate the role of cellular microenvironments, we use novel two-state micropatterns consisting of two adhesion sites connected by a thin stripe. These dumbbell-like micropatterns form a unique framework on which cells are found to repeatedly migrate between the two sites. The assay thus provides numerous time-resolved readouts from

single-cell transitions and yields a population-averaged steady-state distribution of cellular dwell times in each site. The dwell times depend on the area, shape, and orientation of the adhesion sites. We quantify relative cellular preferences and rank absolute escape rates. The simplicity of two-state migration assays provides ample statistics paving the way for applications such as data-driven approaches and cell-based choice assays for biophysical studies.



■ D. B. Brückner, A. Fink, J. O. Rädler, and C. P. Broedersz: *Disentangling the behavioural variability of confined cell migration*; *J R Soc Interface*, 17(163), 20190689 (2020).

Fig. 1. left: Human breast carcinoma cells (MDA-MB-231) in two-state micro-pattern with equal area. **right:** Occupancies depend on area, shape, and orientation.

NONRECIPROCAL DZYALOSHINSKII-MORIYA MAGNETOACOUSTIC WAVES

Matthias Küß, Michael Heigl, Luis Flacke, Andreas Hörner, Mathias Weiler, Manfred Albrecht, and Achim Wixforth

■ https://www.physik.uni-augsburg.de/exp1/mitarbeiter/wixforth_achim/

Surface acoustic waves (SAW) have made their way into both technology and research over the last few decades. They are easily excited and detected on piezoelectric crystals with metal antenna structures and have many different applications, most notably for rf signal processing in telecommunications. As SAWs on piezoelectrics are generally propagating reciprocally, i.e., their properties do not depend on the direction of propagation along a specific crystal axis, the possibility of nonreciprocity would open completely new fields of applications, ranging from acoustic diodes to chiral phononics.

Last year, we studied the interaction of SAWs with spin waves (SWs) in ultra-thin CoFeB/Pt (ferromagnetic/heavy metal) bilayers. Because of SAW-SW coupling mechanisms, such as magnetostriction, the SAW can resonantly excite a SW if the dispersion relations of SAW and SW intersect. Due to the interfacial Dzyaloshinskii-Moriya interaction, the SW dispersion is non-degenerate for oppositely propagating spin waves in

CoFeB/Pt. In combination with the additional nonreciprocity of the magnetoacoustic coupling itself, highly nonreciprocal acoustic wave transmission through the magnetic film is observed. We systematically characterized the magnetoacoustic wave propagation in a thickness series of CoFeB(d)/Pt samples as a function of magnetic field magnitude and direction, and at frequencies up to 7 GHz. Additionally, we quantitatively model our results to extract various magnetic parameters of the magnetic film and thus demonstrate the capabilities of SAW driven SW spectroscopy.

■ M. Küß, M. Heigl, L. Flacke, A. Hörner, M. Weiler, M. Albrecht, and A. Wixforth: *Nonreciprocal Dzyaloshinskii-Moriya Magnetoacoustic Waves*; Phys. Rev. Lett. 125, 217203, <https://doi.org/10.1103/PhysRevLett.125.217203> (2020).

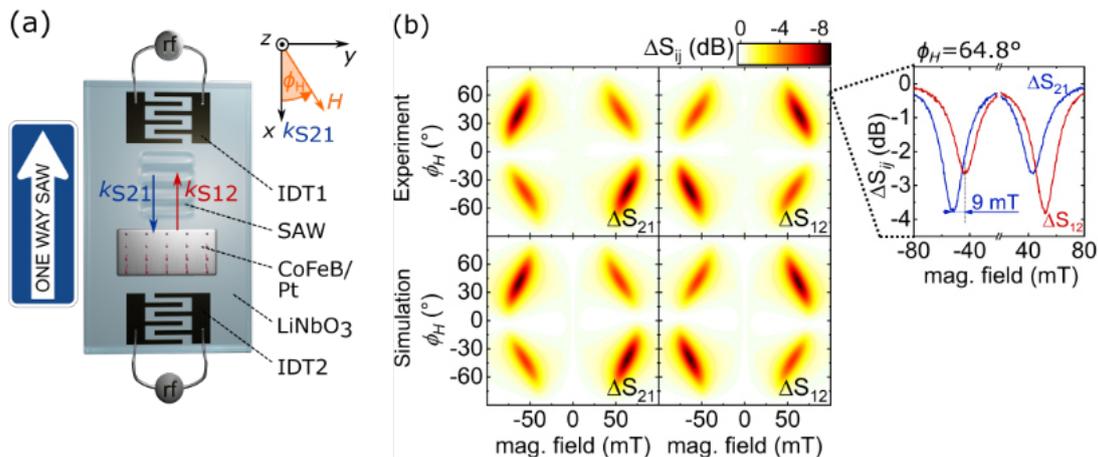


Fig. 1. (a) Schematic illustration of the experimental setup and the coordinate system. Nonreciprocal SAW-SW interaction is characterized by different transmission amplitudes ΔS_{21} and ΔS_{12} for oppositely propagating SAWs k_{21} and k_{12} . (b) Change of the SAW transmission $\Delta S_{ij=21,12}$ as a function of the orientation ϕ_H and magnitude H of the external magnetic field. The experimental ΔS_{21} and ΔS_{12} are measured at the resonance frequencies of the SAW delay lines at 6.9 GHz. The sample reveals nonreciprocal behavior with respect to the transmission magnitude. An additional nonreciprocal shift of the resonance fields is induced by the Dzyaloshinskii-Moriya interaction.

DESIGNED ANCHORING GEOMETRIES DETERMINE LIFETIMES OF BIOTIN-STREPTAVIDIN BONDS UNDER CONSTANT LOAD AND ENABLE ULTRA-STABLE COUPLING

Sophia Gruber, Achim Löff, Steffen M. Sedlak, Martin Benoit, Hermann E. Gaub, and Jan Lipfert

■ <https://www.biophysik.physik.uni-muenchen.de>

■ <https://www.molecularbiophysics.physik.uni-muenchen.de>

The tetravalent protein streptavidin binds the small-molecule biotin (also known as vitamin B7) with extremely high affinity. The biotin-(strept)avidin interaction has served as the biophysical model system for receptor ligand interactions under force, starting with pioneering measurements in the Gaub lab using AFM force spectroscopy (Florin et al., Science 1994; Moy et al., Science 1994) and early molecular dynamics calculations simulating external forces (Grubmüller, et al., Science 1996). On the application side, biotin-streptavidin is ubiquitously used for coupling biological macromolecules in a broad range of diagnostic and single-molecule assays. However, the homotetrameric nature of the streptavidin complex, combined with the fact that streptavidin is often attached unspecifically, means that typically a broad range of force loading geometries are possible. To overcome these limitations, we have engineered streptavidin constructs that can be coupled site-specifically via a cysteine residue and that are engineered so that only defined subunits can bind biotin. We use isothermal titration calorimetry to show that binding to all four subunits is identical thermodynamically. In contrast, when held under constant forces in magnetic tweezers, the lifetimes under force dramatically depend on which subunit is engaged. In the most stable geometry, we achieve a lifetime of ~ 7 h at 65 pN, while the weakest geometry already ruptures on average within ~ 3 min at that force. Our results provide a systematic approach to achieving ultra-stable coupling at the molecular scale and highlight that force stability, unlike thermodynamic stability, depends critically on directionality..

Engineering Anchoring Geometry of Streptavidin

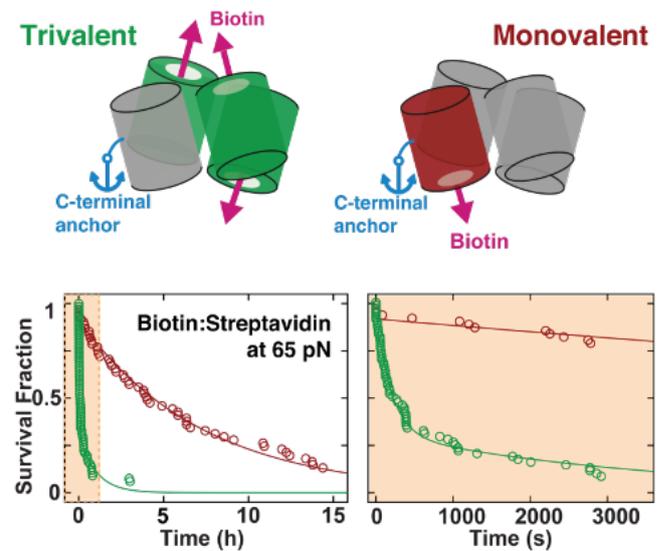


Fig. 1. We engineer streptavidin to control the anchoring geometry and increase the lifetime of the biotin bond under constant force in magnetic tweezers 100-fold. Red shows the monovalent version of the protein that achieves ultra-stable binding under force via the single binding-competent subunit. Green is a version where the other three subunits can bind, giving rise to much shorter and multi-exponential lifetimes.

■ S. Gruber, A. Löff, S. M. Sedlak, M. Benoit, H. E. Gaub, and J. Lipfert: *Designed Anchoring Geometries Determine Lifetimes of Biotin-Streptavidin Bonds under Constant Load and Enable Ultra-Stable Coupling*; *Nanoscale* 12:21131-21137 <https://doi.org/10.1039/D0NR03665J> (2020).

CELL SIZE SETS THE DIAMETER OF THE BUDDING YEAST CONTRACTILE RING

Igor C. Kukhtevich, Nils Lohrberg, Francesco Padovani, Robert Schneider, Kurt M. Schmoller

■ <https://www.helmholtz-muenchen.de/ife/research/kurt-schmoller-cell-and-organelle-size-control/research/index.html>

Cells need to precisely control the amount and size of intracellular structures in response to external and internal cues. Cell size is a major factor determining organelle homeostasis, with the size of many organelles increasing in direct proportion to cell size. However, how biological self-assembly processes set the size of organelles is mostly unclear. Here, we used the budding yeast contractile ring, a well-studied model for self-assembly of subcellular structures, as a model to address this question. Using microfluidics-based live-cell imaging and genetic manipulation of cell size, we found that the diameter of the contractile ring and the bud-neck connecting yeast buds to their mother cells increases with cell volume. Our findings suggest that the ring diameter is set through the dynamic interplay of septin recruitment and Cdc42 polarization during the early stages of bud formation. Importantly, our results provide quantitative predictions that can be used to test models for budding yeast polarization.

■ **I. V. Kukhtevich, N. Lohrberg, F. Padovani, R. Schneider, K. M. Schmoller:** *Cell size sets the diameter of the budding yeast contractile ring*; Nature Communications, 11, 2952 (2020).

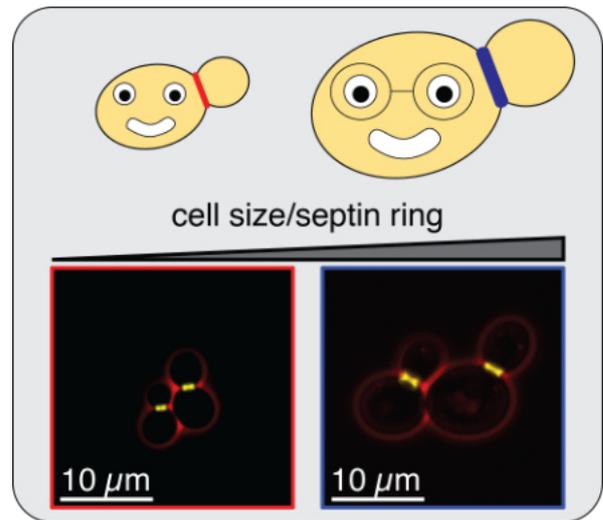


Fig. 1. Cell size determines the diameter of the budding yeast septin & contractile ring.

CELLULAR DELIVERY OF GENOME EDITING CAS9/SGRNA RIBONUCLEO-PROTEIN COMPLEXES VIA OLIGOAMINO AMIDES

Jasmin Kuhn, Yi Lin, Ana Krhac Levacic, Nader Al Danaf, Lun Peng, Miriam Höhn, Don C. Lamb, Ernst Wagner, and Ulrich Lächelt

- <https://www.cup.uni-muenchen.de/pc/lamb/people/lamb.html>
- <https://www.cup.uni-muenchen.de/pb/aks/ewagner/members/dr-ulrich-laechelt/>
- <https://www.cup.lmu.de/pb/aks/ewagner/>

Genome editing provides the opportunity for causal treatments of genetic aberrations with persisting therapeutic effects. The CRISPR/Cas9 system has revolutionized the field of genome editing due to its adaptable endonuclease activity. The functional unit of the system consists of the programmable endonuclease Cas9 and a guide RNA (gRNA), which directs the protein to the target sequence. For therapeutic applications, the genome editing machinery has to be transported into cells, which can be realized using different forms of biomolecules: such as encoding DNA, RNA or as the pre-assembled immediately functional Cas9/gRNA ribonucleoprotein (RNP) complex. Delivery of the complete RNP complex has several advantages over the other approaches, but the delivery of the complex is very challenging.

The article published by Kuhn *et al.* describes the development of a novel platform for the direct cellular delivery of Cas9/sgRNA RNP complexes. A library of cationic lipo-oligomers was generated by

solid-phase synthesis to encapsulate Cas9/sgRNA RNPs in nanoparticles. The nature of the assembly process was identified as ionic interactions between the negatively charged Cas9/sgRNA RNPs and the cationic oligomers. Systematic structural variations showed the lipid-modifications to be important elements that determine the delivery and genome-editing efficiency. The identified best-performing delivery vehicle was well tolerated, transported Cas9/sgRNA RNPs into different cells efficiently, improved endosomal release and mediated gene knock-out at higher levels than a commercially available benchmark reagent. The study demonstrated the potential of the adaptable delivery platform for genome-editing applications.

- **J. Kuhn, Y. Lin, A. Krhac Levacic, N. Al Danaf, L. Peng, M. Höhn, D.C. Lamb, E. Wagner, U. Lächelt:** *Delivery of Cas9/sgRNA Ribonucleoprotein Complexes via Hydroxystearyl Oligoamino Amides*; *Bioconj. Chem.*, DOI: 10.1021/acs.bioconjchem.9b00853 (2020).

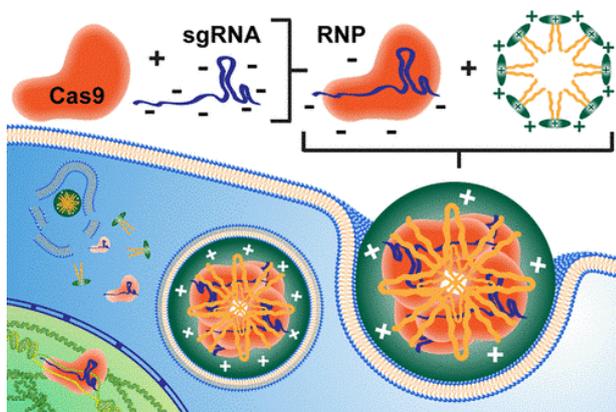


Fig. 1. Schematic illustration of the ionic complex formation between negatively charged Cas9/sgRNA ribonucleoprotein complexes and positively charged lipo-oligomers followed by intracellular delivery.

STRONGLY CORRELATED MATERIALS FROM A NUMERICAL RENORMALIZATION GROUP PERSPECTIVE: HOW THE FERMI-LIQUID STATE OF Sr_2RuO_4 EMERGES

Fabian B. Kugler, Manuel Zingl, Hugo U. R. Strand, Seung-Sup B. Lee, Jan von Delft, and Antoine Georges

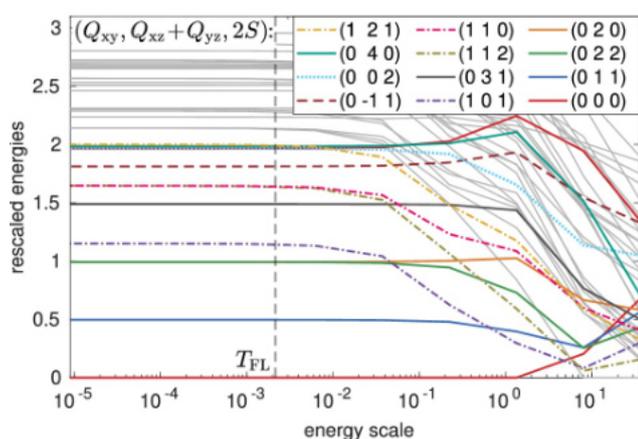
■ <https://homepages.physik.uni-muenchen.de/~vondelft/>

The crossover from fluctuating atomic constituents to a collective state as one lowers temperature or energy is at the heart of the dynamical mean-field theory description of the solid state. Dynamical mean-field theory, as a computational tool, requires an impurity solver that evaluates the local correlations. Since its invention by Wilson in 1975, the numerical renormalization group has proven to be the gold standard for solving simple impurity models, but it was never used in the material context before. In this work, we demonstrate that the numerical renormalization group is indeed a viable tool to monitor the crossover from fluctuating moments to collective behavior in a real-materials setting. We focus on a paradigmatic material of the Hund's metal category, strontium ruthenate, or Sr_2RuO_4 . The renormalization group flow from high to arbitrarily small energy scales, starting from isolated ruthenium atoms, clearly reveals the emergence of the Fermi-liquid state of Sr_2RuO_4 . We find a two-stage screening process, where orbital fluctuations are screened at much higher energies than spin fluctuations, and Fermi-liquid behavior, concomitant with spin coherence, below a temperature of 25 Kelvin. Our work demonstrates the potential of DFT+DMFT+NRG, the combination of density

functional theory, dynamical mean-field theory, and the numerical renormalization group, as a new computational paradigm for real-material systems. It allows us to (i) directly access real-frequency properties at arbitrarily low temperatures and (ii) reveal and elucidate the intricate renormalization process that occurs during the dressing of atomic excitations by their solid-state environment.

■ **F. B. Kugler, M. Zingl, H. U. R. Strand, S.-S. B. Lee, J. von Delft, A. Georges:** *Strongly Correlated Materials from a Numerical Renormalization Group Perspective: How the Fermi-Liquid State of Sr_2RuO_4 Emerges*; Phys. Rev. Lett., doi:110.1103/PhysRevLett.124.016401 (2020).

Fig. 1. Flow diagram of the numerical renormalization group algorithm applied to Sr_2RuO_4 . Going from right to left on the horizontal axis, it describes the system at decreasing energy scales (one electron Volt, or eV, is set to unity). For each energy scale, one sees the rescaled low-energy spectrum, a collection of eigenstates of the many-body Hamiltonian. The legend gives the quantum numbers of each eigenstate in terms of the charge Q in an orbital i , $Q_{_i}$, relative to the ground state, and the total spin S . At high energies, above 10 eV, the system consists of isolated ruthenium atoms favoring large spin due to Hund's coupling. At intermediate energies, below 1 eV, orbital fluctuations get screened by the surrounding atoms and the spectrum undergoes significant changes. For instance, the ground state (lowest red line) emerges as a spin singlet ($S=0$), and the lowest excitation (blue line) is found in the degenerate xz and yz orbitals ($Q_{xz}+Q_{yz}=1$ while $Q_{xy}=0$). At even lower energies, below 0.1 eV, spin fluctuations get screened, as singlet and triplet excitations (orange line with $S=0$ and green line with $S=1$) become degenerate. At the lowest energies, far below 0.01 eV, the system is in its Fermi-liquid state, attested by "towers" of equidistant excitation energies within one symmetry sector (such as the solid lines for excitations in the xz - yz doublet). Indeed, the dashed line indicates an energy of 25 Kelvin, the Fermi-liquid temperature consistently found in experiments.



VIBRATION ENHANCED CELL GROWTH

Manuel S. Brugger, Kathrin Baumgartner, Sophie C. F. Mauritz, Stefan C. Gerlach, Florian Röder, Christine Schlosser, Regina Fluhrer, Achim Wixforth, and Christoph Westerhausen (in collaboration with Hanna Engelke)

■ https://www.physik.uni-augsburg.de/exp1/mitarbeiter/wixforth_achim

■ <https://www.uni-augsburg.de/de/fakultaet/med/profs/physiologie/team/westerhausen/>

In this project, we study a novel approach for enhanced tissue regeneration and wound healing on a chip by utilizing a vibrational stimulation in form of Surface Acoustic Waves (SAW) [1].

Employing live cell imaging, we study the temporal evolution of cell migration in a wound healing assay and compare non-irradiated to irradiated areas on a biochip. We could show that SAW-treated cells exhibit a vigorous increased migration rate.

Moreover, by varying the SAW properties, we demonstrate a clear dependency of the stimulation efficacy on the applied intensity and wave type. Furthermore, by measuring the proliferation, intracellular stress and the exclusion of SAW-related side effects, we can narrow down the cause for increased healing to enhanced cell activity and

migration induced by the mechanical component of the SAW-stimulation.

Current work focuses on the transduction pathway of the acoustic stimulation. Since cells can adapt to mechanical stress by reorganizing the cytoskeletal structure or cell shape, further studies should investigate the impact of known factors that regulate cytoskeletal structure or cell shape. Recently, for instance, an intramembrane protease was implicated in the regulation of protein glycosylation, which strongly impacts the composition of the extracellular matrix and, thus, cytoskeletal structure and cell shape. Another promising intracellular transduction pathway could involve the mechano-sensitive protein yes-associated protein 1.

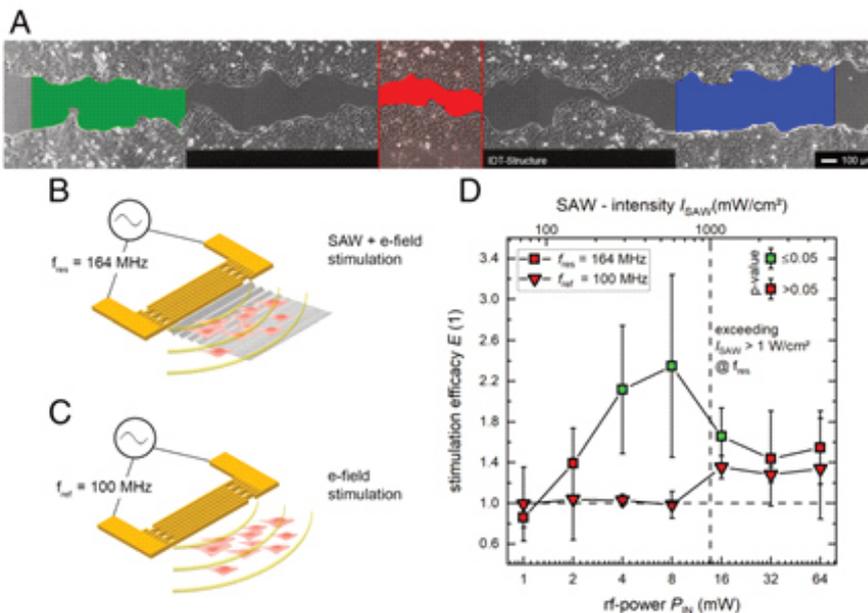


Fig. 1. SAW stimulation of the cell line MDCK-II. (A)

Micrograph of the progressive in vitro wound-healing in a confluent monolayer at $t = 5$ h. The colored regions indicate the SAW-stimulated cells (red) and the internal references (green and blue). **(B and C)** Representations of the different stimuli mechanism at different frequencies. While there is a simultaneous mechanical and electrical stimulation at the SAW resonance frequency, we depict in B the result of an

electrical stimulus only. This is achieved by detuning the IDT frequency to a somewhat lower value outside its bandwidth, where no SAW is excited (C). **(D)** Power dependency on SAW stimulation at different frequencies. There is significant improvement of cell growth and migration rate up to $135 \pm 85\%$ for SAW-supported cell growth at $P_{\text{IN}} = 4$ and 8 mW. Exceeding $I_{\text{SAW}} > 1 \text{ W}/\text{cm}^2$ leads to a decrease of stimulation efficacy E . A significant increase of the efficacy ($P < 0.05$) compared to an external low control is indicated by the color of the symbols' inner area.

Our method offers a powerful platform for future medical treatment, e.g. fast recovery after injury or surgery or the implementation in medical implants as wireless power supplied biochips. This technology can overcome insuperable drawbacks of conventional ultrasound treatment. It provides the opportunity for a widely accessible and cost efficient tissue regeneration treatment option. In addition, employing shear waves in a delay line setup and a much smaller acoustic power, we are able to detect wound healing, changes in adhesion and detachment quantitatively without microscopy [2].

■ **M. S. Brugger, K. Baumgartner, S. C. F. Mauritz, S. C. Gerlach, F. Röder, C. Schlosser, R. Fluhner, A. Wixforth, and C. Westerhausen:** *Vibration enhanced cell growth induced by surface acoustic waves as in vitro wound healing model*; PNAS 117, 31603-31613 (2020).

■ **M. S. Brugger, L. G. Schnitzler, T. Nieberle, A. Wixforth, and C. Westerhausen:** *Shear-Horizontal Surface Acoustic Wave Sensor for Non-Invasive Monitoring of Dynamic Cell Spreading and Attachment in Wound Healing Assays*; Biosensors and Bioelectronics, Vol. 173 (2021) 112807.

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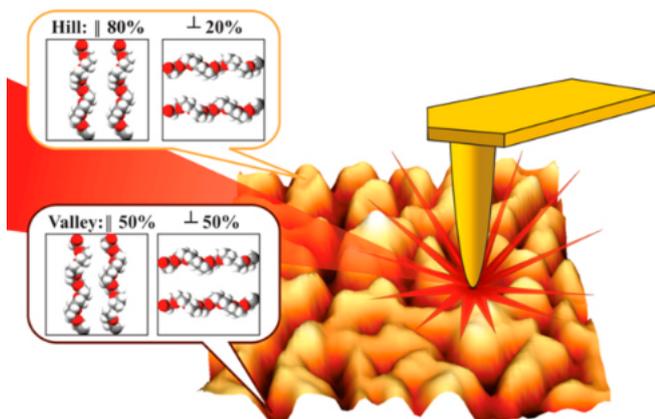
CONFORMATION IN ULTRATHIN POLYMER BRUSH COATINGS RESOLVED BY INFRARED NANOSCOPY

Andres de los Santos Pereira, Adrian Cernescu, Jan Svoboda, Radoslava Sivkova, Iryna Romanenko, Bogdana Bashta, Fritz Keilmann, and Ognjen Pop-Georgievski

■ <https://www.softmatter.physik.uni-muenchen.de/personen/guests/fritz-keilmann1/index.html>

Polymer brush coatings are effective in preventing blood coagulation or bacterial attachment, but their chain conformation, while vital for this effect, was never characterized in high spatial resolution. We report mid-infrared spectroscopic nanoscopy studies of few-nanometer- thin poly(ethylene oxide) (PEO) films which reveal marked spectral variations along the surface at a length scale smaller than 100 nm.

They originate only from the physical conformation of the chains. The conformation and average orientation of the polymer chains in the layer is extracted from the spectra with the aid of theoretical modeling, confirming the spontaneous formation of a crystalline phase. This result suggests spectroscopic nanoscopy as a powerful new tool to characterize polymer brush coatings.



■ **A. Santos Pereira, A. Cernescu, J. Svoboda, R. Sivkova, I. Romanenko, B. Bashta, F. Keilmann, and O. Pop-Georgievski:** *Conformation in ultrathin polymer brush coatings resolved by infrared nanoscopy*; Analytical Chemistry 92, 4716, Doi: 10.1021/acs.analchem.9b05661 (2020).

Fig. 1. Sketch of measuring surface topography and infrared near-field scattering. The insets summarize the different chain orientations in the hills compared to the valleys.

A DNA ORIGAMI PLATFORM FOR SINGLE-PAIR FÖRSTER RESONANCE ENERGY TRANSFER INVESTIGATION OF DNA-DNA INTERACTIONS AND LIGATION

Kira Bartnik, Anders Barth, Mauricio Pilo-Pais, Alvaro H. Crevenna, Tim Liedl, Don C. Lamb

■ https://www.softmatter.physik.uni-muenchen.de/liedl_group/index.html

■ <https://www.cup.uni-muenchen.de/pc/lamb/people/lamb.html>

Measuring molecular interactions using single-molecule techniques is powerful as sample heterogeneities and kinetics can be directly measured, but the experiments require a low concentration of labels. This makes single-molecule experiments inherently difficult when the interactions are weak. Two opposing requirements need to be fulfilled simultaneously: high concentrations of the interaction partners are crucial for weak interactions while, for single molecule measurements, low molecular concentrations are necessary. In this work, we teamed-up with the group of Tim Liedl to develop a DNA origami platform to overcome the aforementioned limitations. We used the DNA-origami platform to study DNA-DNA and DNA-protein interactions in a space-controlled environment with single-pair Förster Resonance Energy Transfer (spFRET). The key findings of our work are: i) The dissociation rate of transient binding scales inversely with the length of the complementary DNA overhang while the association rate is invariant. ii) DNA double-strands with complementary overhangs (sticky ends) are more efficiently ligated by the T4 DNA ligase

than DNA double-strands without complementary overhangs (blunt ends). iii) We could observe the ligation process in real time. We also adapted the system to allow both ligation and restriction enzyme digestion on the same strand. iv) Finally, we followed the transition of a single DNA origami molecule from transient binding of short overhangs to a covalently bound DNA double-strands after incubation with the T4 DNA ligase, followed by a restriction enzyme digestion leading to blunt ends and another ligation step to a double-stranded DNA upon an additional incubation step with the T4 DNA ligase.

This development will help to unravel the dynamics and interactions of weak molecular complexes and to get insights into the existence of subpopulations or detection of rare events, which would otherwise be hidden in ensemble measurements.

■ **K. Bartnik, A. Barth, M. Pilo-Pais, A. H. Crevenna, T. Liedl, and D. C. Lamb:** *A DNA Origami Platform for Single-Pair Förster Resonance Energy Transfer Investigation of DNA-DNA Interactions and Ligation*; *J Am Chem Soc* 142, 815 (2020).

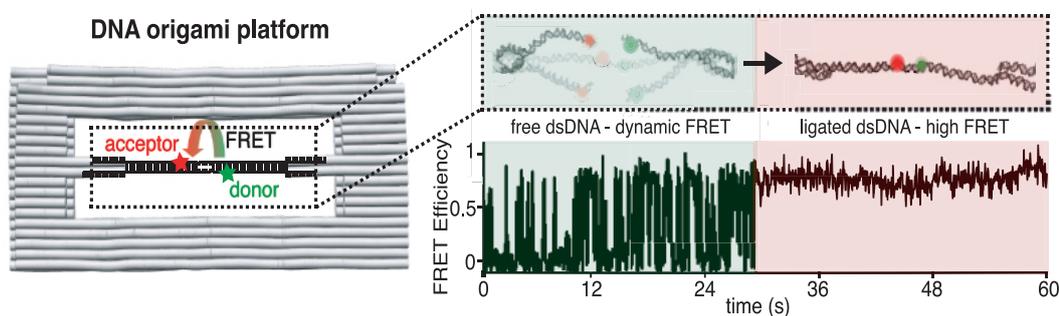


Fig. 1. An origami platform designed to investigate DNA-DNA interactions and DNA ligation. Left: A schematic of the DNA origami platform with a central double-stranded DNA labeled with fluorophores for single-pair Förster Resonance Energy Transfer (spFRET) measurements. Right: Snapshots from a molecular dynamics simulation of the DNA (top) showing conformations on the DNAs before (left side) and after (right side) ligation along with the corresponding spFRET signal (bottom). When small complementary overhangs (sticky ends) are present between the two double-stranded DNA strands, transient interactions between the two strands are observed leading to transitions between a low-FRET and high FRET conformation followed by a stable high FRET signal upon ligation.

SINGLE-VIRUS TRACKING: FROM IMAGING METHODOLOGIES TO VIROLOGICAL APPLICATIONS

Shu-Lin Liu, Zhi-Gang Wang, Hai-Yan Xie, An-An Liu, Don C. Lamb and Dai-Wen Pang

■ <https://www.cup.uni-muenchen.de/pc/lamb/people/lamb.html>

In light of the current pandemic, the importance of understanding viruses and their life-cycle has gained public attention. Viruses are typically smaller than the diffraction limit of optical microscopy, making them difficult to detect. To overcome this limitation, many approaches have been developed for tracking single viruses during the various steps of their life-cycle. In this review article, we summarize the various approaches used for single virus tracking (SVT). SVT is based on fluorescence microscopy and uses the high sensitivity and specificity of fluorescence to follow single viruses during the infection cycle. The group of Lamb has extensive experience in both the fluorescence methodologies used for SVT as well as utilizing SVT to study HIV and Foamy Viruses. Hence, together with the group of Dai-Weng Pang from the University of Nankai, China, they provided a very comprehensive overview of this actual research area.

In this article, the authors give a brief introduction into SVT, the labeling strategies used and mention some of the ground breaking work performed by the early pioneers. They then highlight some of the excellent work that has been done by laboratories around the world to elucidate various steps in the life-cycle of viruses. Lastly, they discuss perspective and future possibilities for SVT.

■ **S.L. Liu, Z.G. Wang, H.Y. Xie, A.A. Liu, D.C. Lamb, and D.W. Pang:** *Single-Virus Tracking: From Imaging Methodologies to Virological Applications*; Chem Rev 120, 1936 (2020).



Fig. 1. This image is from the cover of the *Chemical Review* issue in which this paper was published. It illustrates the various infection pathways that viruses can take. With the aid of single-virus tracing, researcher can elucidate the various interactions between viruses and the host cells during different processes of the viral life-cycle and thereby investigate the mechanisms of viral infection. © Chemical Review 2020.

DESIGN OF BIOCHEMICAL PATTERN FORMING SYSTEMS FROM MINIMAL MOTIFS

Philipp Glock, Fridtjof Brauns, Jacob Halatek, Erwin Frey, and Petra Schwille

■ <https://www.theorie.physik.uni-muenchen.de/lsfrey>

■ <https://www.biochem.mpg.de/de/schwille>

Concentration patterns of proteins in cells control and position important cellular functions such as cell division and cell motility. A well-studied example is the MinDE system of *E. coli*, which produces oscillations of two proteins, MinD and MinE, between the two poles of the cell and thus positions the cell division machinery to midcell. The simplicity of the MinDE system and its reconstitution *in vitro* have been invaluable in understanding the fundamental mechanisms of protein-based pattern formation. Despite its simplicity, the Min proteins are quite complex, both comprising multiple functional domains, responsible for interactions with one another, membrane-binding, switching between different folding conformations and the formation of dimers – pairs of two bound proteins. A key question that remains is whether this structural and functional complexity can be reduced further to reveal a set of minimal ingredients for pattern formation.

We have addressed this question by dissecting MinE into its functional domains. Guided by mathematical modelling, we then synthesized a minimal set of MinE mutants, each comprising only a subset of MinE's functional domains. We then tested the ability of these MinE mutants to form membrane-bound patterns in an *in vitro* setup with MinD and an ATP supply. The core of each mutant is the short helical

sequence of amino acids which MinE uses to interact with MinD. However, this core is not enough to produce patterns. The core needs to be fused with at least one other domain to form patterns. This can either be a membrane-binding domain, or a dimerization domain. Remarkably, neither of these domains needs to be from native MinE, but can be replaced by functional domains from proteins – even from other organisms.

A mathematical model accounting for the biochemical processes mediated by each functional domain reveals that membrane binding and dimerization mediate pattern formation via different self-organizing mechanisms. While membrane binding facilitates recombination of membrane-bound MinE, dimerization drives pattern formation through recruitment-driven cytosolic cycling of MinE. Importantly, numerical simulations show that these mechanisms differ in how the protein pattern aligns relative to the geometry of the rod-shaped *E. coli* bacteria. Only with the dimerization domain, the protein pattern is aligned to oscillate from pole-to-pole, which is key for correct positioning of the cell division machinery.

The modularity and tunability of the MinDE system open the road towards a modular toolbox for protein-based pattern formation. Close collaboration of experiment and theory will facilitate a design-oriented approach to engineer new proteins with tailored functions, sourcing functional domains from different proteins.

■ **P. Glock, F. Brauns, J. Halatek, E. Frey, P. Schwille:** *Design of biochemical pattern forming systems from minimal motifs*; *eLife*, 10.7554/eLife.48646 (2020).

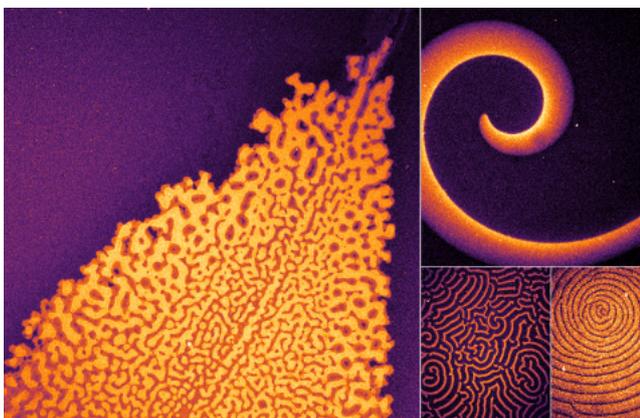


Fig. 1. Fluorescence microscopy images showing a selection of protein patterns formed by the MinDE system with various MinE mutants.

EXCITON g -FACTORS IN MONOLAYER AND BILAYER WSe_2 FROM EXPERIMENT AND THEORY

Jonathan Förste, Nikita V. Tepliakov, Stanislav Yu. Kruchinin, Jessica Lindlau, Victor Funk, Michael Förg, Kenji Watanabe, Takashi Taniguchi, Anvar S. Baimuratov, and Alexander Högele

■ www.nano.physik.uni-muenchen.de

Two-dimensional semiconductors such as WSe_2 have evolved as increasingly significant materials in modern condensed matter research. The growing interest is fueled by the vast diversity of layered crystals that can be thinned down to the ultimate limit of single layers and subsequently reconfigured into artificial solids of rationally designed heterostructures. As such, layered semiconductors represent elementary building blocks for technologies beyond conventional opto-electronics. Despite vital research of the past decade, however, some of the fundamental optical properties arising from excitons in monolayers and bilayers remain controversial.

In this work, we used high magnetic fields to characterize various exciton species in monolayer and bilayer WSe_2 by their respective magneto-induced spectral splitting known as the valley Zeeman splitting. This splitting, proportional to the exciton g -factor, can serve as an unambiguous signature of diverse spin and valley configurations of excitons. Without theory, however, it is merely a phenomenological number. The key aspect of our work therefore was the development of theoretical methods to predict from first principles the exciton g -factors for all possible spin-valley configurations in monolayer and bilayer WSe_2 . By comparing our theoretical predictions with experimental observations, our study conclusively explained some of the controversially debated photoluminescence peaks observed in both layered materials.

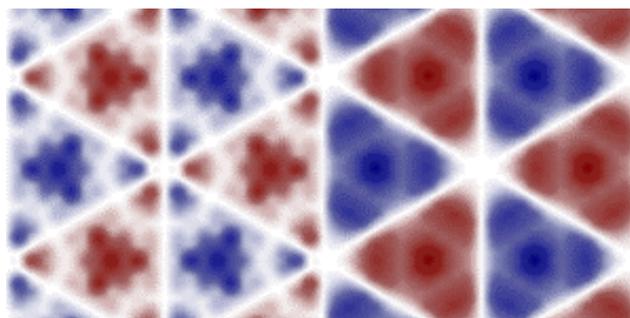


Fig. 1. Orbital angular momenta in the first Brillouin zone for the conduction (left) and valence (right) band states of the bright exciton in monolayer WSe_2 from first principles calculations including spin-orbit effects.

■ **J. Förste, N. V. Tepliakov, S. Yu. Kruchinin, J. Lindlau, V. Funk, M. Förg, K. Watanabe, T. Taniguchi, A. S. Baimuratov, and A. Högele:** *Exciton g -factors in monolayer and bilayer WSe_2 from experiment and theory;* Nat. Commun. 11, 4539 (2020).

HIGH-PRESSURE CO PHASES ON CO(0001) AND THEIR POSSIBLE ROLE IN THE FISCHER-TROPSCH SYNTHESIS

Bernhard Böller, Patrick Zeller, Sebastian Günther, and Joost Wintterlin

■ <https://wintterlin.cup.uni-muenchen.de/>

Unlike most other surface science techniques, scanning tunneling microscopy (STM) is not restricted to a vacuum environment. In principle, it can provide atomically resolved images of catalyst surfaces under the high pressures applied in industry, but practical difficulties have so far prevented a widespread application of STM in high-pressure experiments. In the present study a home-built setup was used, by which layers of adsorbed CO molecules on a cobalt sample were resolved over 12 orders of magnitude in pressure. The study was motivated by the fact that cobalt is the active component of the Fischer-Tropsch catalyst for producing liquid fuels from mixtures of CO and H₂. In previous experiments, performed on a Co(0001) model catalyst at the industrial temperature of ~500 K, adsorbed particles were not resolved, although the surface was covered by a dense monolayer of CO molecules. The high surface mobility of the CO layer at the elevated temperature had prevented resolution. However, when the temperature was reduced to 300 K, a whole series of ordered phases of CO molecules was resolved at CO pressures between 10⁻⁹ and almost 1000 mbar. The figure shows an example at 800 mbar. One can see a long-

range hexagonal superstructure and a hexagonal fine structure from the individual CO molecules. The long-range structure is a moiré effect caused by the fact that the CO molecules formed a hexagonal layer on the hexagonal Co(0001) surface that had a lattice constant that did not match the lattice of the cobalt surface and was also rotated with respect to the surface. At this CO pressure the packing of the molecules was so dense that the particles did no longer bind to defined sites of the cobalt but formed a coherent layer with its own lattice constant. At lower pressures the STM experiments showed CO structures with lower coverages and with other building principles (phase diagram). Because the study covered such a wide range of CO concentrations it could be concluded, by extrapolation to 500 K, that the industrial Fischer-Tropsch synthesis operates in the white, disordered region of the phase diagram.

■ B. Böller, P. Zeller, S. Günther, J. Wintterlin: *High-pressure CO phases on Co(0001) and their possible role in the Fischer-Tropsch synthesis*; ACS Catal., doi 10.1021/acscatal.0c02221 (2020).

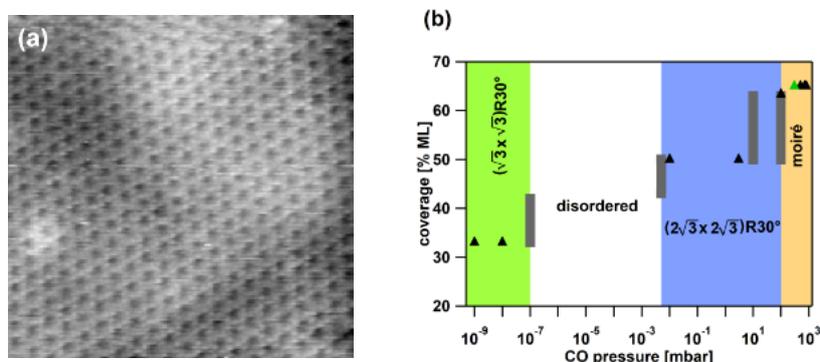


Fig. 1. (a) STM image of a Co(0001) surface covered by a layer of CO molecules. 170 Å x 170 Å. The hexagonal pattern is a moiré structure of the cobalt surface and the CO layer. (b) Phase diagram of all CO structures resolved by STM at 300 K. Adapted with permission from B. Böller, P. Zeller, S. Günther, J. Wintterlin, ACS Catal. 2020, 10, 12156-12166. Copyright 2020 American Chemical Society.

SYNTHESIS ON INERT SURFACES

Markus Lackinger and **Wolfgang M. Heckl**

■ <https://www.deutsches-museum.de/forschung/wissenschaftl-mitarbeiter/pd-dr-markus-lackinger/>

■ <https://www.deutsches-museum.de/wir-ueber-uns/generaldirektor/>

Extended one- and two-dimensional organic nanostructures with intriguing properties are synthesized by direct coupling of functionalized monomers on solid surfaces. In terms of robustness and electronic conjugation, carbon-carbon (C-C) bonded nanostructures are the primary synthetic target. Yet, relevant reactions that afford C-C couplings proceed only on metal surfaces that are, however, inappropriate for electronic applications. Accordingly, generally applicable approaches for synthesis on the chemically inert surfaces of insulators are highly desirable. To this end, a conceptually straightforward approach is proposed: deposition of pre-generated polyradicals that can readily form C-C bonded nanostructures by radical addition on arbitrary surfaces, whose chemical contribution is then no longer required. Therefore, a radical deposition source (RDS, (a)) was devised, where halogenated precursors are indirectly deposited through a heated reactive drift tube. A gold coating on its surface renders the tube mildly reactive to facilitate the conversion of the precursors into radicals by dehalogenation upon transient adsorption. The en route generated radicals are guided to the end of the tube by sequences of adsorption-desorption processes, where they effuse for subsequent deposition. In a proof-of-principle experiment the iodinated precursor 4,4''-diiodo-p-terphenyl (DITP) was studied on metal surfaces that

were passivated with a closed densely packed monolayer of iodine. Upon deposition of the DITP derived terphenyl biradicals self-assembled structures of monomers were observed (b), which spontaneously recombine into covalently bound dimers (sexiphenyl biradicals, (c)) at room temperature. Progressive coupling into extended poly-para-phenylene (PPP, (d)) wires required additional thermal activation for breaking bonds between radicals and iodine atoms of the passivation layer, but no further chemical activation.

■ **G. Galeotti, M. Fritton, and M. Lackinger:** *Carbon-Carbon Coupling on Inert Surfaces by Deposition of en Route Generated Aryl Radicals*; *Angew. Chem. Int. Ed.*, 10.1002/anie.202010833 (2020).

■ **G. Galeotti, M. Fritton, and M. Lackinger:** *Kohlenstoff-Kohlenstoff-Kupplung auf inerten Oberflächen durch die Abscheidung von en route erzeugten Aryl Radikalen*; *Angew. Chem.*, 10.1002/ange.202010833 (2020).

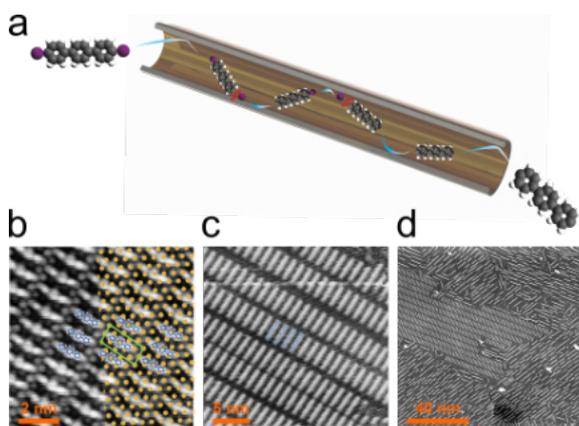


Fig. 1. On-surface synthesis by direct deposition of radicals. a Scheme of the deposition through the mildly reactive gold-coated drift tube of the radical deposition source (RDS). Halogenated 4,4''-diiodo-p-terphenyl (DITP) precursors are deposited through the tube (left hand side). Its hot surface catalyzes the dissociation of iodine-substituents and guides the so generated terphenyl biradicals through the tube, where they effuse at the end (right hand side) for downstream deposition. b – d Scanning Tunneling Microscopy (STM) images acquired after deposition of biradicals generated from DITP precursors onto iodine-passivated Ag(111) and Au(111) surfaces; The initially observed highly organized structures of b terphenyl and c sexiphenyl biradicals (spontaneously formed at room temperature) grew into d more extended PPP wires after mild heating. This STM image shows a prevailing ordered domain of sexiphenyl biradicals at the center left. Panels b-d adapted from 10.1002/anie.202010833 under the terms of the Creative Commons CC BY license.

DNA STRANDS TRIGGER THE INTRACELLULAR RELEASE OF DRUGS FROM MUCIN-BASED NANOCARRIERS

Ceren Kimna, Theresa M. Lutz, Hongji Yan, Jian Song, Thomas Crouzier, and Oliver Lieleg

■ <https://www.professoren.tum.de/lieleg-oliver>

Gaining control over the delivery of therapeutics to a specific disease site is still very challenging. However, especially when cytotoxic drugs such as chemotherapeutics are used, the importance of a control mechanism that can differentiate “sick” target cells from the surrounding healthy tissue is pivotal. Here, we designed a nanoparticle-based drug delivery process, which releases an active agent only in the presence of a specific trigger DNA sequence. With this strategy, we were able to initiate the release of therapeutics into the cytosol with high efficiency. Furthermore, we demonstrated how an endogenous marker (e.g., a specific miRNA sequence) that is overexpressed in the initial phases of certain cancer types can be used as a stimulus to autonomously initiate intracellular drug release - and only in such cells, where this pathophysiological marker is present. We expect that this precisely controlled delivery mechanism can facilitate the design of site-specific treatments for such diseases, where an overexpression of signature oligonucleotide sequences has been identified.

■ C. Kimna, T. M. Lutz, H. Yan, J. Song, T. Crouzier, and O. Lieleg: *DNA Strands Trigger the Intracellular Release of Drugs from Mucin-Based Nanocarriers*; ACS Nano DOI: 10.1021/ac-nano.0c04035 (2020).

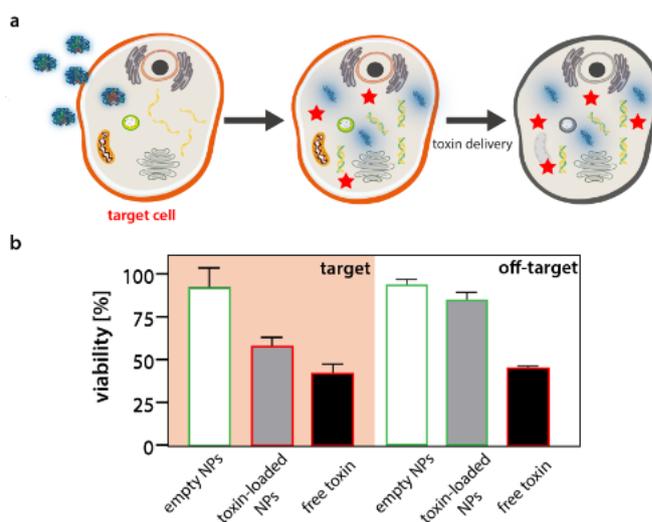


Fig. 1. (a) Schematic representation of the targeted delivery approach. Cellular miRNA overexpressed in the target cells acts as a trigger, which opens the condensed, drug-loaded mucin nanoparticles (NPs) by selective hybridization with the NP-stabilizing DNA strands. As a consequence, the drug is released into the cytosol of those target cells. (b) In vitro viability of target (HeLa) and off-target (NIH/3T3) cells as determined 24 h after uptake of toxin-loaded NPs (n = 9). Only the cells holding the correct trigger (i.e., overexpressed miRNA) can initiate the autonomous drug release (which leads to cell death). Data shown represents mean values, error bars denote the standard deviation.

SODIUM DODECYLBENZENE SULFONATE INTERFACE MODIFICATION OF METHYLAMMONIUM LEAD IODIDE AS SURFACE PASSIVATION OF PEROVSKITE SOLAR CELLS

Yuqin Zou, Renjun Guo, Buyruk Ali, Wei Chen, Tianxiao Xiao, Shanshan Yin, Xinyu Jiang, Lucas P. Kreuzer, Cheng Mu, Tayebeh Ameri, Matthias Schwartzkopf, Stephan V. Roth, Peter Müller-Buschbaum

■ <https://www.cup.lmu.de/pc/ameri>

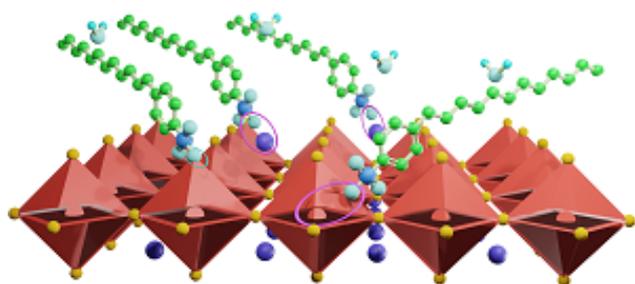
■ <https://www.groups.ph.tum.de/polymer/peter-mueller-buschbaum/>

Perovskite solar cells (PSCs) have been developed as a promising photovoltaic technology due to their impressive optoelectronic properties. However, the long-term stability under ambient conditions in terms of thermal load, light, oxygen, and moisture exposure greatly limits its commercial application. Generally, the instability of PSCs mainly arises from the inherently unstable nature of perovskite materials caused by component degradation, defect states, and under-coordinated cations and anions (I^- , MA^+ and Pb^{2+}). The commonly used methylammonium (MA^+) cation has relatively poor stability and is prone to degrade and volatilize, resulting in a deterioration of the active layer components. Additionally, the free lead ions have low formation energy and accumulate at the surface and grain boundaries, which is considered to be one of the main sources of defect states.

To effectively improve the longevity of the device and passivate the detrimental defects accumulating at the grain boundaries and at the surface of the perovskite thin films, we incorporate the functional ligand sodium dodecylbenzene sulfonate (SDBS) into the

perovskite component to functionalize the surface. The negatively charged sulfonic groups of SDBS can form complexes with uncoordinated Pb^{2+} and MA^+ existing on the surface of the film (Figure 1). The electrostatic interaction between $-SO_3^-$ and MA^+ causes the hydrophilic sulfonic group of the SDBS molecules to face the inside of the perovskite film, resulting in a decrease of the surface tension between the hole transport layer (HTL) and the active layer, and increase the adhesion. Due to the steric effects, the hydrophobic long alkyl chain aggregated on the surface of perovskite film will point to the outwards for resisting the infiltration of external moisture, which improves the stability of the active layer components under humid ambient conditions. As a result, outstanding stability and superior photovoltaic properties devices can be achieved.

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A DIFFUSIOPHORETIC MECHANISM FOR ATP-DRIVEN TRANSPORT WITHOUT MOTOR PROTEINS

Beatrice Ramm, Andriy Goychuk, Alena Khmelinskaia, Philipp Blumhardt, Hiromune Eto, Kristina A. Ganzinger, Erwin Frey, and Petra Schwille

■ <https://www.theorie.physik.uni-muenchen.de/lsfrey>

■ <https://www.biochem.mpg.de/de/schwille>

Cells must ensure that molecular cargoes are delivered in a timely manner to their intended destinations in order to perform their biological functions. To do so, cells employ sophisticated transport mechanisms that are usually based on specific interactions, where energy-consuming motor proteins convey cargo to its destination. In a joint effort between experiment and theory, we have uncovered an additional mode of transport driven by pattern-forming reaction-diffusion systems. Specifically, we investigated the *E. coli* MinDE reaction-diffusion system, a model for self-organized pattern formation that has been studied in depth for nearly 20 years. It has been widely believed that the sole purpose of the oscillations generated by MinDE in the cell is the positioning of the FtsZ inhibitor MinC at the cell poles, constraining FtsZ to midcell. While recent experiments have shown that the MinDE system can also regulate other unrelated membrane-bound proteins by non-specific means, the broader biological implications, and more importantly, the underlying physics remained elusive.

To close this gap and explain how MinDE patterns may induce active transport of biomolecules, we set up a highly controllable *in vitro* platform. We reconstituted MinDE pattern formation on artificial membranes and generated a modular synthetic cargo: a DNA-origami scaffold with multiple streptavidin building blocks. Using these nanostructures, we demonstrated that transport depends on the effective size of the cargo and that MinDE can even sort molecules according to size. These highly controllable experiments allowed us to determine the underlying transport mechanism by means of a theoretical analysis. We found that the experiments can only be explained by diffusiophoresis, driven by non-equilibrium currents of ATP-consuming active proteins. Such non-equilibrium currents naturally occur in pat-

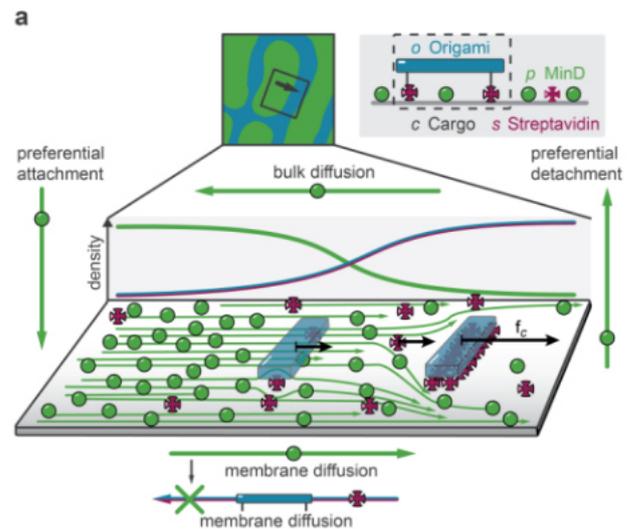


Fig. 1. Schematic of our theoretical model. Reactions and diffusion of MinDE proteins generate MinD (green) surface density gradients. On the membrane, diffusive MinD fluxes (green arrows), exert a frictional force (black arrow) on the cargo molecules (blue origami scaffold with magenta streptavidin building blocks). As a result, a cargo molecule gradient builds up. In steady state, thermodynamic forces (entropic repulsion and mixing, which drive cargo diffusion) balance the frictional force that is exerted by protein flows. Figure reproduced from <https://doi.org/10.1038/s41567-021-01213-3> under the CC-BY 4.0 License.

tern-forming systems in the form of reactive currents that build up gradients and diffusive currents. In our case, diffusive currents on the membrane couple to the cargo via an effective mesoscopic friction, thus driving diffusiophoretic transport. Diffusiophoresis was first described by Derjaguin 50 years ago and has long been demonstrated to occur in colloidal suspensions. With other physicochemical mechanisms such as liquid-liquid phase separation taking the spotlight in biology, diffusiophoresis could represent a new kind of generic transport mechanism in cells never described so far in biological settings. This mechanism could be especially important in

simpler biological systems, such as prokaryotes and early life forms, as they lack(ed) the highly complex motor proteins present in higher organisms.

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SLOW TRANSITION PATH TIMES REVEAL A COMPLEX FOLDING BARRIER IN A DESIGNED PROTEIN

Alexander Mehlich, Jie Fang, Benjamin Pelz, Hongbin Li, and Johannes Stigler

■ <https://www.genzentrum.uni-muenchen.de/research-groups/stigler>

De-novo designed proteins have received wide interest as potential platforms for nano-engineering and biomedicine. While the field has made significant progress in the efficient design of thermodynamically stable proteins, the folding process of artificially designed proteins is not well-studied. We used single-molecule force spectroscopy by optical tweezers to study the folding of ROSS, a de-novo designed protein that adopts a 2x2 Rossmann fold. Unexpectedly, we found that the time for crossing the energy barrier separating the unfolded and folded states (the transition path time) is in the millisecond range, much slower than what has been reported for other systems. While long transition path times can be explained by barrier roughness or slow diffusion, we could show that isotropic roughness cannot explain the measured transition path time distribution. Instead, we could demonstrate that the slow barrier crossing of ROSS is caused by the population of three short-lived high-energy intermediates. This has unexpected consequences, such as an unintuitive increase of transition path times at higher tension. In addition, we identified incomplete and off-pathway folding events with different barrier crossing dynamics. Our results hint at the presence of a complex rugged transition barrier that may be a common feature of many artificially designed proteins.

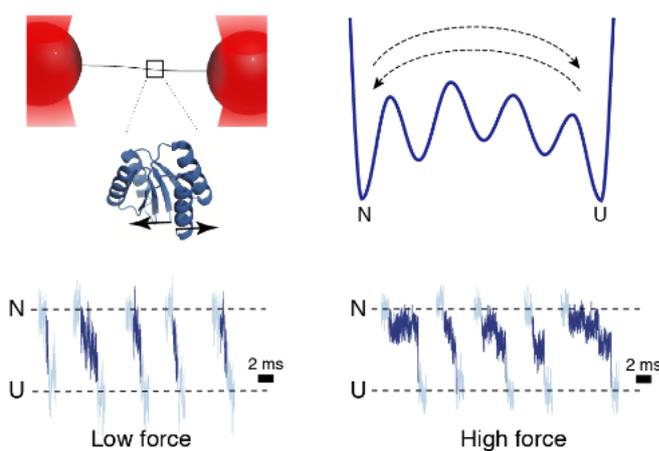


Fig. 1. A designed 2x2 Rossmann fold protein has an unusually rugged folding energy barrier separating the native (N) and unfolded (U) state. The experimentally determined barrier crossing time is among the slowest reported so far. High-energy intermediates lead to unintuitive consequences, such as slowed barrier crossing times at higher force.

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IMMUNOGENICITY OF CAS9 PROTEIN

Aditi Mehta, and Olivia M. Merkel

■ <https://www.cup.lmu.de/pb/aks/merkel>

Clustered regularly interspaced short palindromic repeats (CRISPR) form the adaptive immune system in archaea and bacteria and have been modified for genome engineering in eukaryotic cells. CRISPR systems contain 2 components, a single-guide RNA, which is a short RNA composed of a 20 nucleotide sequence that targets specific sites in the genomic DNA and a scaffold necessary for its binding to the CRISPR-associated endonuclease (Cas9). Because of its high efficiency and accuracy, the CRISPR-Cas9 genome editing based therapies are poised to treat a multitude of human diseases with a promise to target previously “undruggable” proteins. As the first in-body clinical trial with CRISPR-Cas9 is embarked on, the risks associated with administering the genome editing machinery to patients become increasingly relevant. Recent studies have demonstrated an innate and adaptive cellular immune response to Cas9 in mouse models and the presence of anti-Cas9 antibodies and T-cells in human plasma. Pre-existing immunity against therapeutic Cas9 delivery could decrease its efficacy in vivo and may pose significant safety issues. This review focuses on the immunogenicity of the Cas9 protein and summarizes potential approaches to circumvent the problem of immune recognition.

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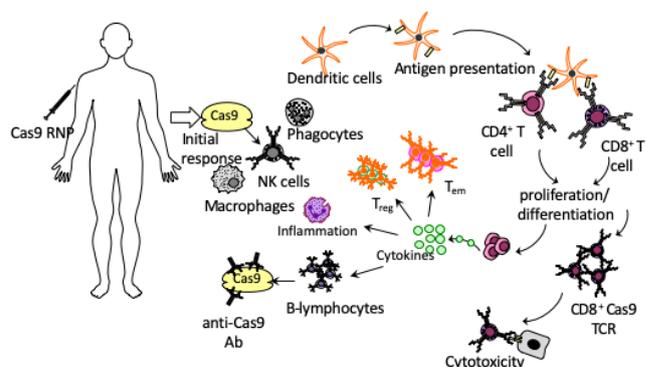
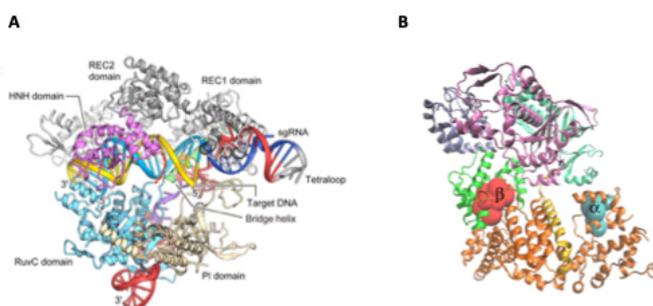


Fig. 1. The immune response to Cas9. Injection of CRISPR machinery triggers an innate and adaptive immune response.



ternary complex. Ribbon representation of the Cas9-sgRNA-DNA complex. Disordered linkers are shown as red dotted lines. Reproduced with permission from. **(b)** 3-D structure of the SpCas9 protein, showing the location of the identified immunodominant epitopes α and β . Reproduced with permission from Mehta & Merkel, Journal of Pharmaceutical Sciences (2020).

ELUCIDATING THE PERFORMANCE LIMITS OF PEROVSKITE NANOCRYSTAL LIGHT-EMITTING DIODES

Thomas Morgenstern, Carola Lampe, Tassilow Naujoks, Matthew Jurow, Yi Liu, Alexander S. Urban, and Wolfgang Brütting

■ <https://www.nanospec.physik.uni-muenchen.de/>

One of our research focuses is the synthesis and fundamental understanding of two-dimensional lead halide perovskite nanoplatelets (NPLs). With this study, we looked to extend our research scope. We had previously fabricated CsPbBr₃ NPLs, whose emission is shifted to the blue spectral region through quantum confinement, and incorporated these in electroluminescent devices (LEDs). While these constituted some of the best-performing devices at the time, their overall efficiency (EQE) was still relatively low, and we wanted to understand whether this was a general limitation of the NPLs. In collaboration with Wolfgang Brütting at the University of Augsburg, we conducted a study to investigate how the dimensionality of the NPLs affects the outcoupling from a working LED. For this, we simulated the radiation patterns emanating from thin films of NPLs with thicknesses ranging from 2 monolayers up to nanocubes. The confinement in one dimension leads to preferential orientation of the

exciton and the resulting light emission. This orientation becomes pronounced with increasing confinement in the NPLs. Accordingly, while the maximum EQE achievable with nanocubes is only 20%, this value increases to 28% for the thinnest NPLs. One of the main problems affecting the NPLs is the low photoluminescence quantum yield, and accordingly, the total EQE would be limited to only 15% without an improvement in this respect. Nevertheless, this study shows how beneficial the anisotropy of the perovskite NPLs can be and offers a guide for further improvement of semiconductor nanocrystal-based LEDs.

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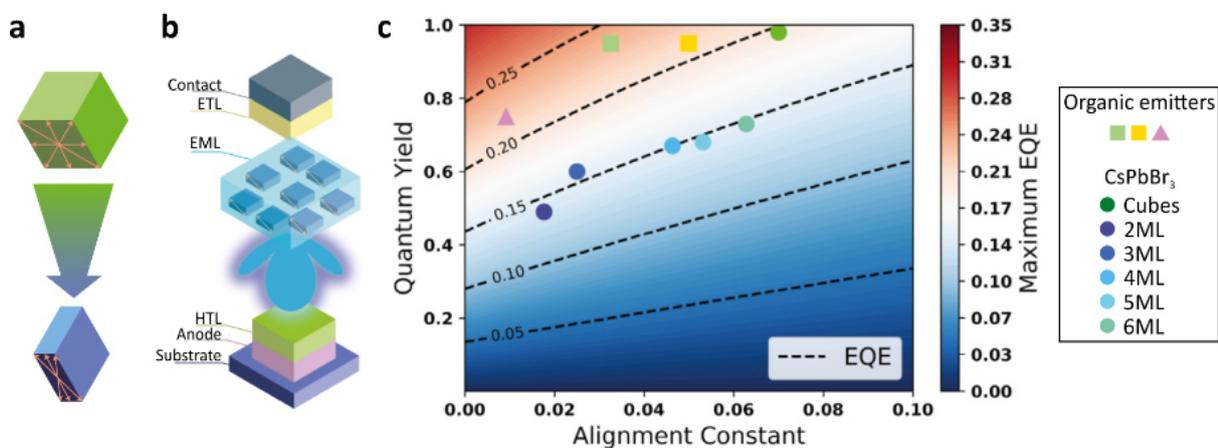


Fig. 1. Alignment of the transition dipole in perovskite nanoplatelets enhances LED efficiency. **a)** With increasing confinement in perovskite NPLs, the transition dipole becomes more strongly oriented. **b)** The NPLs and their respective radiation patterns are simulated in a full working LED stack. **c)** The alignment constant determines the maximum EQE attainable, reaching nearly 30% for the NPLs, thus far outperforming nanocubes and widespread blue-emitting organic molecules.

HIGHLY CONDUCTING WURSTER-TYPE TWISTED COVALENT ORGANIC FRAMEWORKS

Julian M. Rotter, Roman Guntermann, Michael Auth, André Mähringer, Andreas Sperlich, Vladimir Dyakonov, Dana D. Medina, Thomas Bein

■ <https://bein.cup.uni-muenchen.de>

Covalent organic frameworks (COFs) define a versatile structural paradigm combining attractive properties such as crystallinity, porosity, and chemical and structural modularity which are valuable for various applications. For the incorporation of COFs into optoelectronic devices, efficient charge carrier transport and intrinsic conductivity are often essential. Here, the authors report the synthesis of two imine-linked two-dimensional COFs, WTA and WBDT, featuring a redox-active Wurster-type motif based on the twisted tetragonal N,N,N',N'-tetraphenyl-1,4-phenylenediamine node. By condensing this unit with either terephthalaldehyde (TA) or benzodithiophene dialdehyde (BDT), COFs featuring a dual-pore kagome-type structure were obtained as highly crystalline materials with large specific surface areas and mesoporosity. In addition, the experimentally determined high conduction band energies of both COFs render them suitable candidates for oxidative doping. The incorporation of a benzodithiophene linear building block into the COF allows for high intrinsic macroscopic conductivity. Both anisotropic and average isotropic electrical conductivities were determined with van der Pauw measurements using oriented films and pressed pellets, respectively. Furthermore, the impact of different dopants such as F₄TCNQ, antimony pentachloride and iodine on the

conductivities of the resulting doped COFs was studied. By using the strong organic acceptor F₄TCNQ, a massive increase of the radical cation density (up to 0.5 radicals per unit cell) and long-term stable electrical conductivity as high as 3.67 S m⁻¹ were achieved for the anisotropic transport in an oriented film, one of the highest for any doped COF to date. Interestingly, no significant differences between isotropic and anisotropic charge transport were found in films and pressed pellets. This work expands the list of possible building nodes for electrically conducting COFs from planar systems to twisted geometries. The achievement of high and stable electrical conductivity paves the way for possible applications of new COFs in organic (opto)electronics.

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THESES



Santiago Aguirre: Multiloop functional renormalization group in the Keldysh formalism - A study of the single-impurity Anderson mode (LMU, von Delft)

Fabian Apfelbeck: Growth, Characterization and Transfer of Highly-Ordered Organic Semiconductor Thin Films (LMU, Liedl)

Nico Arlt: Dynamics of the antisymmetric Lotka-Volterra equation (LMU, Frey)

Felix Bangerter: Tensor Hypercontracted Second Order Møller-Plesset Perturbation Theory (LMU, Ochsenfeld)

Anna Baptist: Using ASAXS as a Molecular Ruler in Proteins (LMU, Lipfert)

Alexander Battenberg: Evolutionary dynamics of fitness model with neutral axis (LMU, Frey)

Nina Beier: Setup for Combined Magnetic Tweezers Studies and Total Internal Reflection Microscopy (LMU, Lipfert)

Lina Beisswenger: Hybridization of covalent organic framework photoabsorbers with molecular co-catalysts (LMU, Lotsch)

Benedikt Bichler: High Energy Transmission Synchrotron X-ray Diffraction for Thermal Diffuse Scattering Research of MAPbBr₃ Single Crystals (LMU, Liedl)

Katharina Biechele: Zustandsdiagramme der Wirkstoffaufnahme in lebende Zellen (Universität Augsburg, Westerhausen)

Florian Binder: Engineering Poly(heptazine Imides) as Potential Photocatalysts for the Nitrogen Reduction Reaction (LMU, Lotsch)

Felix Brandner: Investigation of Topology Dependent DNA Binding of SYBR Gold (LMU,

Lipfert)

Julia Brunkert: Effective theories for pseudogap metals (LMU, Punk)

Gintare Budryte: Soft robotics based on thermo-responsive polymeric thin films (TUM, Müller-Buschbaum)

Robert Calaminus: Phase Engineering in Thiophosphate Solid Electrolytes: Lithium Argyrodite Formation in Li₇SiPS₈ (LMU, Lotsch)

Pauline Chotard: Printed organic solar cells (TUM, Müller-Buschbaum)

Cindy Close: Advancing DNA Origami Plasmonic Nanoantennas for Biosensing at the Single-Molecule Level (LMU, Tinnefeld)

Fiona Cole: Nutzung der Fluoreszenzlebensdauerinformation in gepulster MINFLUX Nanoskopie; Simultaneous Localisation of Two Emitters on Sub-Diffraction Length Scales by Pulsed-Interleaved MINFLUX Nanoscopy (LMU, Tinnefeld / TUM, Hauer)

Juri Crimmann: Elucidating the Synthetic Process, Morphology, and Optical Properties of Micellar Perovskite Nanocrystals (LMU, Urban)

Gianni Del Bimbo: Dynamical Mean-Field Theory + Numerical Renormalization Group Study of Strongly Correlated Systems with Spin-Orbit Coupling: (LMU, von Delft)

Lautaro Diaz Piola: Morphology study of water-processed active layers for hybrid photovoltaic applications (TUM, Müller-Buschbaum)

Maximilian Dorfner: A hybrid NRG-DMRG approach to spectral properties of an Anderson impurity embedded in a BCS superconductor (LMU, von Delft)

Anxiang Ge: Analytic Continuation of Correlators from the Matsubara to the Keldysh Formalism (LMU, von Delft)

Thomas Eisenreich: Deep-Spots: Spot Detection and Classification with Neural Networks (LMU, Wöhrstein)

Florian Fink: Synthesis and characterization of transition metal doped 2D layered materials based on $ZrSe(x)Te(2-x)$ and Ti_2PTe_2 (LMU, Lotsch)

Tim Fürmann: Influence of Anisotropy on the Photocatalytic Activity and Charge Carrier Dynamics in Thickness-Controlled BiOX Nanosheets (LMU, Feldmann)

Dmitry German: Studies on the Non-linear Optical Interactions of Particles-on-Mirror Systems with a Pulse Shaping Setup (LMU, Hartschuh)

Georg Glänzer: Interfaces between polymer electrolyte, electrodes and metal current collectors of thin film lithium-ion batteries (TUM, Müller-Buschbaum)

Nina Gordon: Investigation of asymmetries in plasmonic nanoantenna-controlled back focal plane patterns (LMU, Hartschuh)

Florian Goschin: Spectroscopic Temperature Measurements on the Nanoscale (LMU, Cortés)

Christoph Gruber: Implementation of an interferometric scattering microscope for imaging nanoscopic processes in perovskite nanomaterials (LMU, Cortés)

Juan Guerrero: Reaction-diffusion systems on dynamically evolving surfaces (LMU, Frey)

Adina Hausch: Force Spectroscopy of von Willebrand Factor in the Low-Force Regime (LMU, Lipfert)

Stefan Heiserer: Optical Spectroscopy of 2D-layered Perovskites (LMU, Feldmann)

Johannes Heyn: Time Lapse Analysis of Nuclear Positions and Cell Mechanics in Single-Cell Migration on 1D Micropattern (LMU, Rädler)

Rico Holfeuer: In-situ analysis of the formation and evolution of (LMU, Bein)

Lukas Horndasch: Protein NMR with Thymine DANN Glycosylase (TDG) (LMU, Rovó)

Linus Huber: Effect of temperature on the morphology and device performance of printed nonfullerene acceptor based organic solar cells (TUM, Müller-Buschbaum)

Henrik Intat: Critical Variable Selection as a Feature Selection Method for Single-Cell RNA Sequency Data (LMU, Rädler)

Fabian Knechtel: Characterization of a Newly Built Confocal Laser Scanning Microscope and its Usage to Investigate Different Organic Light Emitting Diodes (LMU, Lamb)

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Center for NanoScience (CeNS)
Ludwig-Maximilians-Universität
Geschwister-Scholl-Platz 1
D-80539 Munich, Germany
Phone: +49-89-2180-3547
[v www.cens.de](http://www.cens.de)

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