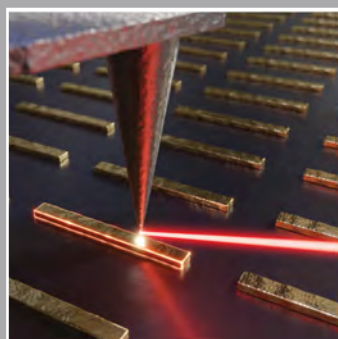
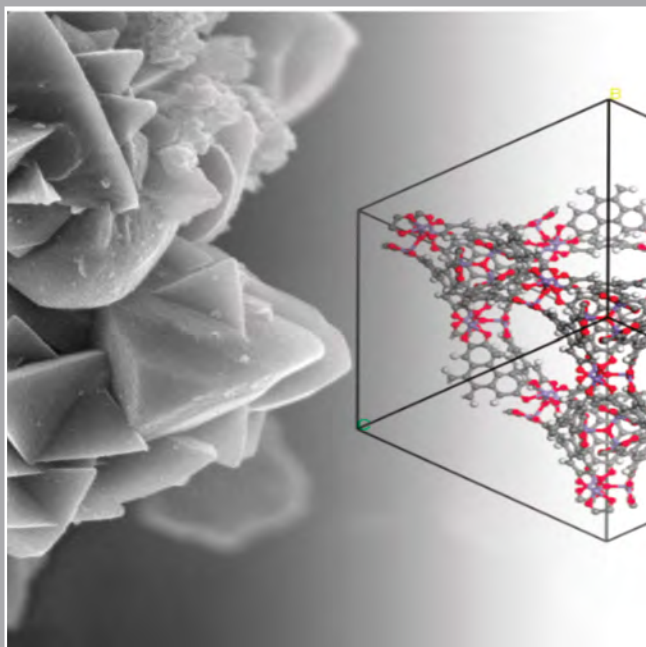


CENTER FOR NANOSCIENCE ANNUAL REPORT 2021



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CENTER FOR NANOSCIENCE
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In 2021, CeNS went hybrid. With the arrival of covid vaccination during the first half of the year, corona protection measures evolved into a cluttered body of legislation. CeNS activities,

which had been restricted to Zoom sessions for more than a year, gradually moved back to in-person meetings with others joining virtually. Thanks to the CeNS management team and the support of Christian Hundschell, hybrid meetings became the new normal. It is great to see that the CeNS community can get through difficult times without losing its optimism, passion for science and cooperative spirit.

The Scientific Advisory Board was reelected and three new Board Members, Atac Imamoglu, Tanja Weil and Naomi Halas agreed to support us. We would like to express our gratitude to the departing member, Klaus Müllen, who served as a member of the advisory board for more than 20 years. We are also happy to welcome our new CeNS members Dana Medina, Knut Müller-Caspary, Evelyn Plötz, Benedikt Sabass, and Sabine Schneider. There has also been some change in the CeNS office: Claudia Leonhardt left the team after almost 10 years. We are grateful to her for her dedicated work, always with a smile on her face, and wish her all the best for her new endeavours at MCQST.

Two of our CeNS spin-offs, attocube systems and ibidi GmbH, celebrated their 20th anniversary in 2021. We send them our best wishes for the next 20 years and our gratitude for their continued support of the Nano Innovation Award.

To foster early independence and academic careers, CeNS launched the Young Investigator Funds last year. Five postdoctoral researchers received EUR 5,000-10,000 of funding. We hope that these funds will help our early career researchers to build successful careers as future leaders in nanoscience.

Despite the difficult circumstances, CeNS organized a variety of events, many of them virtual, including the kick-off event for the initiative Engineering Life at LMU, "CeNS meets Industry", the workshop "NanoScience for Future" and the PhD event "Responsible Research", to mention just a few. In addition, members of CeNS and MCQST gathered for a joint poster session in September 2021 as one of the first larger live events since the start of the pandemic.

Last but not least, on the initiative of the CeNS student representatives and the CeNS board, a PhD survey on supervision and leadership was carried out in cooperation with the GraduateCenter-LMU. The survey provided us with honest and valuable feedback about students' expectations of PhD project management, supervision and communication. In the course of further discussions at the CeNS Annual Assembly, the idea of a PhD Ombudsperson at CeNS was brought up, and we are extremely grateful that Hermann Gaub volunteered to establish this role.

We hope that the reader finds interest in this annual report with remarkable scientific contributions and refreshing ideas. We would like to thank all who contributed and helped us to enjoy the science of nanoscience.

*Prof. Joachim Rädler
Board Member of CeNS*

NEW MEMBERS

Dr. Evelyn Plötz LMU Munich



Evelyn Plötz studied physics at LMU Munich and the Université Paris XI - Sud, Orsay. She received her PhD degree from LMU Munich for her thesis on "Spectral modulations in Femtosecond Stimulated Raman Microscopy (FSRM)" at the

Chair for BioMolecular Optics (Wolfgang Zinth / Peter Gilch). In 2011, she joined the lab of Thorben Cordes as a postdoctoral fellow at the RU Groningen before she returned to LMU Munich as a postdoctoral fellow in the lab of Don Lamb at the chemistry department in December 2015.

Since 2017, Evelyn has been a junior group leader for chemically sensitive (single-molecule) imaging. Her research focuses on developing correlative imaging and spectroscopy methods for advanced material characterisation. Currently, she combines various label-free, optical methodologies with high spatiotemporal resolution, including coherent Raman, multi-photon and nonlinear processes, to follow the uptake and interaction with porous materials at the molecular and particle level.

Dr. Dana Medina LMU Munich



Dana Medina-Tautz obtained her Ph.D. in Chemistry in 2010 from Bar-Ilan University (Israel). In 2011, Dana moved to the Ludwig-Maximilians-Universität München (LMU, chair Prof. Thomas Bein) as a Minerva fellow to conduct postdoctoral research, where she is cur-

rently leading a young research group and working towards her habilitation. The research pursued by Dana's group focuses on the design and synthesis of functional porous crystalline frameworks, particularly 2D layered structures. A large part of the research is dedicated to the development of novel on-surface deposition techniques with the goal of bringing periodic porous materials towards thin film applications in electronics, sensing and sieving.

Prof. Knut Müller-Caspary LMU Munich



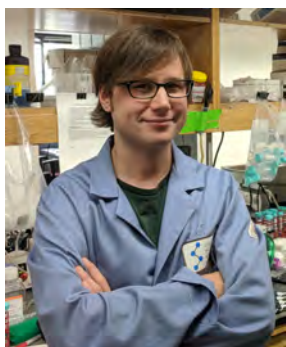
Since 2021, Knut Müller-Caspary has been a W2 Professor for Transmission Electron Microscopy of Nanostructures, at LMU's Faculty of Chemistry and Pharmacy. After his Ph.D. on "Transmission electron microscopy of semiconductor nanostructures using ab-initio

structure factors for strain-relaxed supercells" and a subsequent postdoctoral period at Bremen University, he moved to the Institute for Electron Microscopy in Materials Science (EMAT) at the Universiteit Antwerpen in Belgium in 2016. In 2018, he became group leader of the moreSTEM group within the framework of a Helmholtz Young Investigator Group fellowship at Forschungszentrum Jülich, dedicated to multidimensional ultrafast TEM, and joined the RWTH Aachen Physics Faculty as a (junior) professor in 2019. Müller-Caspary's TEM experience covers the fields of quantitative aberration-corrected TEM and STEM, electron diffraction and spectroscopy as well as simulation and methodological developments. His recent research interests focus on the development and application of multi-dimensional (S)TEM for electrical characterisation of functional nanostructures at subatomic scales, in-situ heating and biasing experiments at atomic resolution, high-contrast imaging of soft and biological

matter at low-doses, and phase retrieval by electron ptychography and artificial intelligence.

Dr. David Konrad

LMU Munich



David Konrad studied chemistry and biochemistry at the Ludwig Maximilian University (LMU) Munich and received his M.Sc. in 2013. During his master's studies, he worked as a visiting researcher in the group of Dean Toste at the University of California, Berkeley

and the group of Benjamin List at the Max Planck Institute for Coal Research in Mülheim a. d. Ruhr. In 2014, David joined the group of Dirk Trauner for his graduate studies to work towards an asymmetric synthesis of tetrodotoxin and methods to red-shift photopharmaceuticals. After graduating in 2018, David moved to the Scripps Research Institute in La Jolla as a postdoctoral fellow under the guidance of Benjamin Cravatt. As part of the return phase of his fellowship, David joined the group of Ivan Huc at the Department of Pharmacy of LMU Munich, where he became a group leader funded by a Liebig fellowship in 2021. His research interests include: redshifted photoswitchable nanoagents, synthetic methodologies, drug development, chemical proteomics, and non-small cell lung cancer.

Prof. Benedikt Sabass

LMU Munich



Benedikt Sabass has been a W2 Professor for Cell Biophysics and Statistical Physics at LMU's Faculty of Veterinary Medicine and Faculty of Physics since 2020.

After a Diploma in Physics from Heidelberg University and a PhD in

Theoretical Physics at Stuttgart University (in the

group of Udo Seifert), Prof. Sabass worked in industrial R&D on the project "intelligent Zero Emission Urban System" for PORSCHE AG for one year. After deciding to return to academia, he spent a brief period of time at Heidelberg University in the Group of Ulrich Schwarz before moving to Princeton University, where he worked as a postdoctoral researcher with Howard A. Stone. From 2016 to 2020, he was a group leader at Forschungszentrum Jülich at the Institute of Biological Information Processing. A theoretical physicist by training, he is inspired by the beauty and effectiveness of biological mechanisms. His work revolves around topics from cell biology and fundamental questions in theoretical biophysics, combining theory and experimental work in the laboratory.

Dr. Sabine Schneider

LMU Munich



Sabine Schneider studied Biology at LMU Munich, with a diploma thesis in the group of Michael Stürzl, GSF Research Centre for Environment and Health, Neuherberg. From 2004 to 2007, she worked on her PhD in the group of Max Paoli, University of Nottingham

and Griffith University Brisbane, Australia. After her PhD, she returned to Germany as a postdoctoral fellow in the group of Thomas Carell. From 2010 to 2019, Dr. Schneider was a group leader at the Department of Chemistry, TU Munich. Since 2019, she has been a Heisenberg fellow and research group leader at LMU's Department of Chemistry. Her research focuses on structure-function relationship of nucleic acids, how they interact and modulate protein function and recognize small molecules, using molecular biology, biochemistry and X-ray crystallography.

CENS ADVISORY BOARD



Prof. Naomi Halas, Rice University, USA, became a new member of the CeNS Advisory Board.



Prof. Atac Imamoglu, ETH Zürich, Switzerland, became a new member of the CeNS Advisory Board.



Prof. Tanja Weil, MPI for Polymer Research Mainz, became a new member of the CeNS Advisory Board.

CALLS & APPOINTMENTS



PD Dr. Tayebbeh Ameri (LMU) became Senior Lecturer (Associate Professor) in the Institute for Materials and Processes, Chemical Engineering discipline at the University of Edinburgh.



PD Dr. Ulrich Lächelt (LMU) was appointed associate professor at the Division of Pharmaceutical Technology and Biopharmaceutics at the University of Vienna.



Prof. Jan Lipfert (LMU) was appointed as Full Professor in Experimental Biophysics & Bio-Inspired Materials at the University of Utrecht (The Netherlands).



Dr. Jacek Stolarczyk (LMU) was appointed as a professor at the Jagiellonian University in Krakow (Poland).

AWARDS & GRANTS



Prof. Emiliano Cortés was featured as a "2021 Emerging Investigator" by J. Mat. Chem. A.



Prof. Olivia Merkel (LMU) was awarded an ERC Proof of Concept Grant 2021 for her project "Novel Asthma Therapy".



Prof. Wolfgang M. Heckl (TUM & Deutsches Museum) received the Arthur Burkhardt-Preis from the Arthur-Burkhardt Foundation.



Dr. Andreas Tittl (LMU) received the STEMM Global Award Prize at the Conference on Smart NanoMaterials, Paris, France.



Prof. Hermann Gaub (LMU) was honoured as a member of the 2021 Class of Fellows of the Biophysical Society.



Prof. Ernst Wagner (LMU) received an Honorary Professorship from Jinan University, China.



Prof. Jan Lipfert (LMU) received the teaching prize of the Faculty of Biology ("Bio-Plus") and the teaching prize of the Faculty of Chemistry and Pharmacy ("Preis für gute Lehre").

From Capturing Viruses to Bioprinting - Nano Innovation Award 2021



Three doctoral researchers from Munich were awarded the 2021 Nano Innovation Award by the Center for NanoScience. The prize for innovative research in applica-

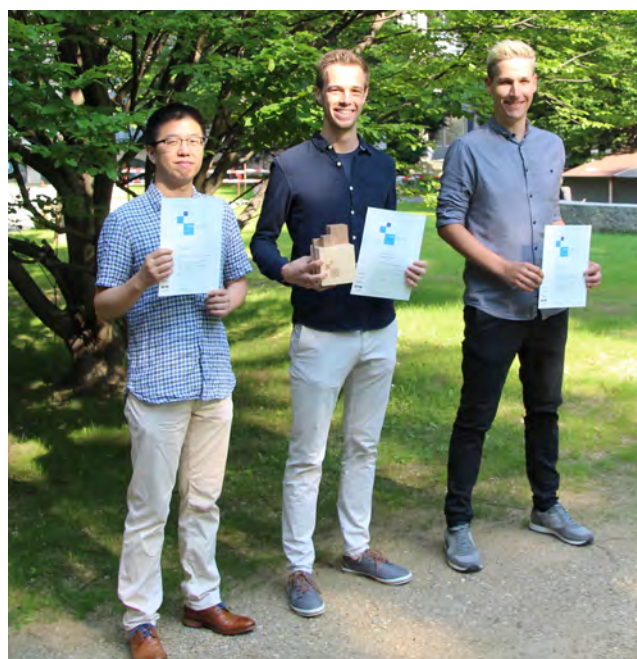
tion-oriented nanosciences is worth €9,000. An expert jury from industry and academia selected the winners from applicants from throughout Bavaria

While most science prizes honour excellent results in basic research, the Nano Innovation Award focuses on high innovation and application potential. The companies attocube systems, ibidi, Nanion Technologies and NanoTemper Technologies, together with CeNS, award the prize to talented and creative young scientists whose results are not only of interest for basic research but also promise future technological applications.

The **first prize** went to **Christian Sigl from TU Munich**, who developed the molecular basis for an unconventional antiviral concept. His work is based on the idea of enclosing whole viruses in macromolecular shells that block the molecular interactions between virus and host cell. The DNA origami platform he developed for this purpose offers a promising approach for combating different viruses using the same concept. The shells developed by Christian provide the technical basis for the interdisciplinary EU consortium VIROFIGHT, which will further test and develop the new therapeutic concept.

The jury awarded **second place** to **Jan Felber from LMU Munich**. In his work, he succeeded for the first time in creating cell-selective redox sensors for disease-relevant reductases (a specific group of enzymes). His work opens up a broad spectrum of possible applications in biomedicine, from basic research and use in drug development to clinical diagnostics and therapeutics. Jan Felber has already launched several transfer projects, e.g. a start-up for the development of therapeutics and a collaboration with Tubulis GmbH for a novel and powerful linker for antibody-drug conjugates.

Jun Zhang from Munich University of Applied Sciences secured the **third place** with a novel bioprinting technology that can transfer cells from a reservoir to a target substrate with very high precision using ultra-short laser pulses. By integrating the setup into an inverted optical microscope, it becomes possible to preselect individual cells from complex cell mixtures. The potential applications are manifold - from fundamental questions in cell biology, to single-cell



From left to right: Jun Zhang, Christian Sigl, and Jan Felber.

analysis methods, to the production of organ-on-a-chip and tissue engineering. A BMBF-funded project is now developing a user-friendly, fully automated system based on Jun Zhang's findings.

Four former CeNS spin-offs, attocube systems, ibidi, Nanion Technologies and NanoTemper Technologies, have been supporting the award since 2015. "For ibidi, CeNS is a constant source of inspiration through technological and personal exchange and an important link to the scientific community. This year, the work submitted for the Nano Innovation Award once again was characterized by exceptionally high creativity and quality. Congratulations to the winners and all participants!", said Roman Zantl, co-founder and managing director of ibidi and a member of the jury this year.

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

CeNS Young Investigator Fund

To promote the scientific independence of postdoctoral researchers, CeNS has launched the CeNS Young Investigator Fund. The CeNS Young Investigator Fund comes with up to €10,000 to support the postdocs' own research projects. From all nominations, the CeNS board selected five recipients based on the innovative and creative nature and the interdisciplinary character of their work, as well as the potential shown by the candidate as a future leader in nanoscience.

Dr. Viktorija Glembockyte has been a postdoc in the group of Prof. Tinnefeld for 3 years and she is transitioning to establish her own junior research group. Her research focuses on the development of fluorescence-based diagnostic assays based on plasmonic DNA origami nanoantennas, succeeding in detecting single DNA molecules that can indicate antibiotic resistance on a battery-powered smartphone microscope.

Dr. Martin Reynders is a postdoctoral researcher in chemical biology and biophysics in the group of Dr. Oliver Thorn-Seshold. Despite his early career stage, he has acquired years of practical experience from project design to synthetic chemistry, cell biology, biochemistry, and even optics/electronics. This experience now puts him in an ideal position to build interdisciplinary projects, with the broader vision to direct the generation of new tools and therapeutics based on smart molecules that mimic and surpass the abilities of enzymes.

Dr. Jenny Schneider has been working in the group of Prof. Thomas Bein since 2020. Her research is focused on understanding the mechanistic steps involved in green fuel generation via solar-to-chemical energy conversion. For example, Dr. Schneider has developed a smart design of the electrode/molecule interface that allows the identification of the parameters affecting light-induced interfacial electron transfer kinetics and (photo)catalysis.

Dr. Ana Sousa Castillo gained international experience and visibility, working in many different groups and countries around the world, before joining the group of Prof. Emiliano Cortés at LMU. She is currently developing and tuning hybrid nanomaterials to enhance the efficiency with which sunlight can be converted into chemical energy and fuels.

Dr. Juan Wang joined the group of Dr. Andreas Tittl in 2020. Since then, she has developed a new research direction within the group to overcome the application limits of current nanophotonic biosensors. Specifically, she is working to combine a unique nanophotonic approach (top-down all-dielectric metasurfaces united with bottom-up metallic nanoparticles) with microfluidic technology, enabling an entirely new class of on-chip sensor devices with strong diagnostics and clinical applications. www.cens.de/research/cens-young-investigator-fund/

Responsible Research

What is responsible research? How can I present data accurately and reproducibly? What about preprint publishing and how does this change the conventional publication routines? What do I need to know about open science? What is the link between mental health, well-being and responsible research? What is an ombudsman and why should we discuss responsible conduct of research in the global context? – These and more questions were covered at the “Responsible Research” online event in March 2021. To raise awareness of this important topic, CeNS teamed up with graduate programs in the greater Munich area and the GraduateCenterLMU to organize a campus-wide educational event.

More than 300 participants had access to an interactive online platform for keynote lectures with Professor Ernst Winnacker, Professor Ulrich Dirnagl and others, breakout sessions and meet-the-speaker forums, active breaks and interactive participation such as polls, feedback rounds and more. The feedback from the participants showed that the topic and format were

well received: “Great and inspiring talks and stimulating discussions. Excellent meeting format in Corona times.”

www.responsibleresearch.graduatecenter.uni-muenchen.de/event2021

Engineering Life Initiative – Kick-off and new seminar series

On April 8, the Engineering Life Initiative (eLi) at LMU Munich started with an official Kick-off event. Scientists from CeNS, the LMU Gene Center and the LMU Arnold Sommerfeld Center for Theoretical

Physics have joined forces to combine novel physics-centered experimental methods, system-level computational approaches, and conceptual bottom-up theory to decipher the physical laws governing the dynamic organization of life from molecules to cells. The aim is to advance the understanding of the physics of living systems across scales and to re-engineer life-like processes and systems by employing state-of-the-art technologies and by developing novel life-inspired approaches. At the virtual Kick-off event, renowned speakers Cees Dekker, Tanja Kortemme, Barbara Treutlein and Michael Elowitz discussed questions such as “What is life – The bottom-up route?” and “Multicellular circuit design” and addressed fundamental questions of the research field in the subsequent panel discussion.

After this truly inspiring start, eLi has now established a regular biweekly seminar series with external speakers on Thursdays at 5.00 pm.

www.engineering-life.de

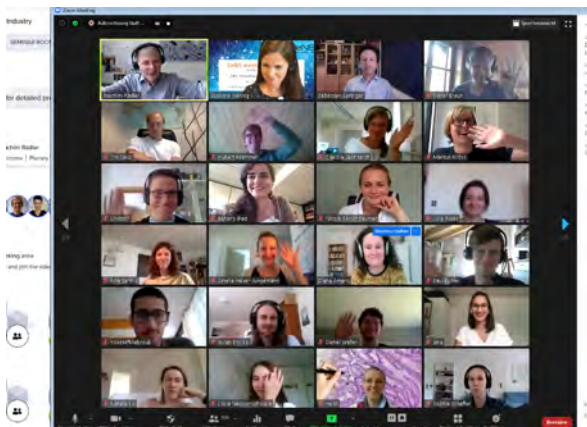
Girl's Day 2021

In April 2021, CeNS welcomed 15 girls for a virtual "One day as a nanoscientist". In several short sessions, the girls learned about nanoscience in general and saw demonstrations of current research within CeNS, such as fluorescence detection with a smartphone, DNA origami, and Atomic Force Microscopy. They also took part in virtual lab tours and inspiring discussions with role models - female students and scientists at different career stages, from master studies to independent group leader. The program was rounded off by several interactive quiz sessions. The online setting enabled girls from more distant places in Bavaria to join the program – a real opportunity to spread promote interest in science and nanoscience in particular outside Munich.

www.girls-day.de

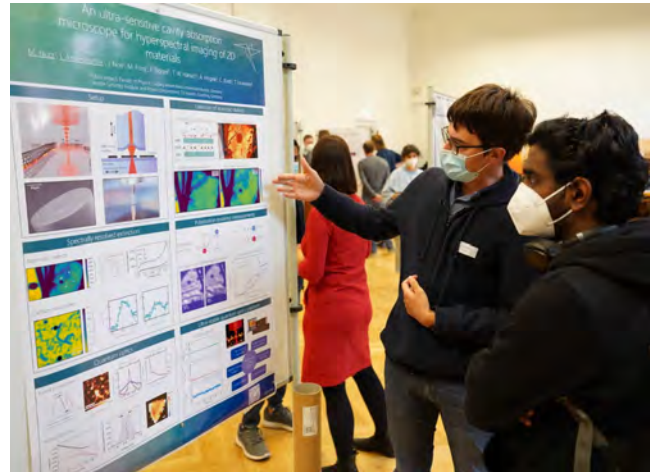
CeNS meets Industry

At this online event, CeNS fostered the exchange between academic and industrial research. Invited speakers from companies such as Wacker AG, Bruker Scientific, ibidi GmbH, and IQM Quantum Computers presented their work, their company and their professional career. Afterwards, the speakers and other company representatives were available at virtual company booths to answer individual questions. In pandemic times, the format proved to be very valuable and attractive, especially for PhD students planning their next career step. www.cens.de/calendar/workshops-events/cens-meets-industry-2021/



Nano meets Quantum

In September 2021, it was finally possible to hold in-person events again. Researchers from CeNS and the Munich Center for Quantum Technologies met for a poster session at LMU to exchange research ideas and present their results. The large number of attendants and posters showed the importance of and desire for in-person meetings and live discussions.



Science in a Nutshell

Organized by the CeNS Student Representatives 2021, Pauline Kolbeck, Michael Scheckenbach, and Simone Ezendam, the annual event "Science in a Nutshell" featured three exciting talks on different research areas of CeNS. Annalena Salditt (AG Braun) spoke on "Origin of life in a rockshell? - How physics can help prebiotic chemistry". Sina Stocker (AG Reuter) came all the way from Berlin to present "Machine learning and its applications to materials science". Last but not least, Prof. Christian Planck's talk (ethris GmbH) on "Development of mRNA therapeutics for lung disease" showcased a very current topic.

"Science in a Nutshell" is also the official annual welcome event for all new CeNS junior members. More than 50 graduate students and post-docs used the opportunity to join a live event again and meet their peers from CeNS.

NanoScience for Future

The current climate crisis requires the identification of new directions of research and political actions. Not only is a closed carbon cycle necessary, but also means to reduce CO₂ directly. Together with the Center for Advanced Studies (CAS) at LMU, CeNS initiated an online event “Scientific Background on Emissions and Carbon Dioxide Removal” where nanoscientists explored carbon dioxide removal options together with geoscientists and a stakeholder from Siemens Energy. After an introduction to the carbon budget and the need for CO₂ removal by Prof. Julia Pongratz (LMU Geosciences), Prof. Andreas Oschlies (GEOMAR Kiel) discussed marine and technological CO₂ removal options. Dr. Volkmar Pflug from Siemens Energy complemented the academic perspective with industrial examples of direct air capture to produce climate-neutral fuels. The event thematically supplemented the “Energy of the Future” event series organized by the Cluster of Excellence e-conversion together with the CAS in 2021, focusing on sustainable energy use and production.

Frontiers in Physics of Life

In November, the Physics of Life community within CeNS held an online symposium on “Frontiers in Physics of Life”. The eight speakers covered a wide range of biophysical topics, including DNA-based super-resolution microscopy (Ralf Jungmann), engineering of cell-free genetic systems (Hannes Mutschler), physical mechanisms of chromatin condensation (Jan Brugues), chromosomes as memory machines (Leonid Myrni), mechanisms of epithelial tissue morphodynamics (Margaret Gardel), and different topics of mechanobiology such as mechanobiology of intestinal organoids (Xavier Trepate), mechanical control of cell plasticity and error correction in the early embryo (Verena Ruprecht), and dissecting the link between signalling and mechanics (Guillaume Charras).

Transferable Skills Workshops

CeNS continued to offer a variety of transferable skills workshops to its graduate students and postdocs, especially during times where access to the labs was still restricted. Topics included Job Applications, Scientific Writing and Publishing, Python, 3D Graphical Design, Research Data Training, and Project Management for Scientists.

attocube systems



20 years ago, attocube was founded as a spin-off from CeNS. The company develops, produces and distributes components and systems for nanoscale applications such as precision motion, cryogenic microscopy, and nanoscale analytics. All products are manufactured in the NanoFactory, the company's headquarters in Haar, close to Munich. Today, attocube is a leading pioneer for nanotechnology solutions in industry and research. An international team of 150 physicists, engineers, software developers, and product designers work in close collaboration from conception through to delivery.

Attocube, together with their technology partner WITec, won a 2021 Innovation Award from The Analytical Scientist for their cryoRaman. The cryoRaman - jointly developed by attocube and WITec - integrates attocube's leading-edge cryostat and nanopositioner technology with the much-vaunted sensitivity and modularity of WITec's correlative microscope series. For the first time, Raman imaging at the lowest temperatures in high magnetic fields is easily accessible with unmatched spatial, spectral and depth resolution.

Source: www.attocube.com

ethris

Ethris' lead COVID-19 therapeutic candidate, ETH47, has been awarded "The Most Innovative Product Top 3" in the category of Leap Innovations at the Pharma Trend Image &

Innovation Awards 2021. Ethris was eligible to apply for the prize after having received a research grant from the State of Bavaria in Germany for the development of its COVID-19 therapy. ETH47 is a therapeutic candidate that harbours the mRNA blueprint for type III interferon. It is designed to be administered directly to the respiratory tract to treat early infection caused by SARS-CoV-2 and its variants by activating the innate immune system, and therefore stopping infection before the onset of severe symptoms.

Source: www.ethris.com

IBIDI



In 2021, ibidi celebrated its 20th anniversary. Within two decades, ibidi has succeeded in becoming the world's leading provider of products for cell-based microscopy assays. Today, ibidi is a medium-sized company with headquarters in Munich (Germany) and Madison, Wisconsin (USA), a strong network of



ibidi founders: Joachim Rädler, Roman Zantl, Valentin Kahl, and Ulf Rädler (left to right)

global distribution partners, over 500 products, and more than 40,000 customers worldwide.

For its excellent crisis strategy during the pandemic, ibidi GmbH has been awarded the Export Award Bavaria 2021: Special Edition 2021, in the category "Successful Order Processing in Corona Times". The award, which has been presented since 2007 to small- and medium-sized companies that work with foreign markets, this time recognizes the unique travel and supply chains challenges caused by the Corona virus in 2020.

Source: www.ibidi.com

NanoTemper Technologies

NanoTemper has been given 2021's TOP 100 seal, an award that honours innovative German small and medium-sized companies. The TOP 100 innovation competition is organized by compamedia, and judging is led by innovation researcher Prof. Dr. Nikolaus Franke and his team. They assess companies using around 120 test criteria from five categories: innovation-friendly senior management, innovation climate, innovative processes and organization, outward looking innovation, and successful innovations. The panel also looked to see that innovation is the result of a planned approach (i.e., repeatable innovative performance) and that solutions succeed on the market. Due to the current global pandemic, this round also examined the entrepreneurial response to the COVID-19 crisis.

Source: <https://nanotempertech.com>



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- 5 **Structured Sequences Emerge from Random Pool when Replicated by Templated Ligation** (Dieter Braun et al.) 24
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BIFUNCTIONAL PASSIVATION OF MAPbI₃ PEROVSKITE SOLAR CELLS

Achim Hartschuh, Peter Müller-Buschbaum, Thomas Bein, and Tayebbeh Ameri

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Defects created at the surface and grain boundaries of polycrystalline hybrid-halide perovskite thin films significantly deteriorate the photovoltaic performance and stability of corresponding devices. Passivation of these defects with appropriate ligands appears to be one of the most promising concepts to address this issue. We implemented 1,10-phenanthroline, known as a bidentate chelating ligand, between the MAPbI₃ film and the hole-transport layer for both passivating lead-based surface defects and converting the excess/unreacted lead iodide (PbI₂) buried at interfaces, into “neutralized” and beneficial species. We verified the defect healing ability of 1,10-phenanthroline in a collaborative effort using a broad set of complementary spectroscopic techniques. In addition, we analysed the structure and chemical composition at the perovskite surface after treatment at nanoscale spatial resolution by high-angle annular dark-field scanning transmission electron microscopy and nano-Fourier transform infrared (nano-FTIR) spectroscopy (figure 1b). On

the basis of our experimental results, we conclude that 1,10-phenanthroline treatment induces the formation of different morphologies with distinct chemical compositions on the surface of the perovskite film such that surface defects are effectively passivated, and excess/unreacted PbI₂ is converted into beneficial complex species at the modified interface (figure 1a). As a result, an improved power conversion efficiency (20.16%) and significantly more stable unencapsulated perovskite solar cells are obtained with the 1,10-phenanthroline treatment compared to the MAPbI₃ reference device (18.03%).

■ A. Buyruk, D. Blätte, M. Günther, M. A. Scheel, N. F. Hartmann, M. Döblinger, A. Weis, A. Hartschuh, P. Müller-Buschbaum, T. Bein, and T. Ameri: *1,10-Phenanthroline as an Efficient Bifunctional Passivating Agent for MAPbI₃ Perovskite Solar Cells*; ACS Appl. Mater. Interfaces, DOI: 10.1021/acsami.1c05055 (2021).

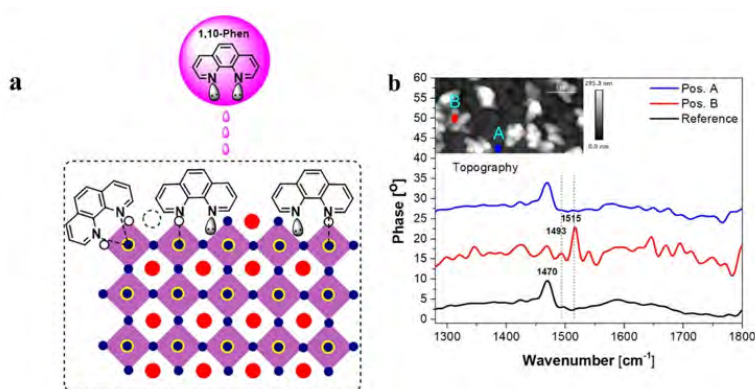


Figure 1. (a) Schematic illustration of the bifunctional surface passivation of MAPbI₃ by 1,10-phenanthroline. (b) Nano-FTIR spectra of untreated MAPbI₃ (reference) and 1,10-phen-treated films for two different sample positions (A, B) marked in the topography scan (inset). The peaks at 1515 and 1493 cm⁻¹ are identified as the vibrational IR-active modes of PbI₂ (1,10-phen)_x (x = 1, 2) with different relative contributions.

MESOPOROUS SILICA NANOPARTICLES AS PH-RESPONSIVE CARRIER FOR THE IMMUNE-ACTIVATING DRUG RESIQUIMOD ENHANCE THE LOCAL IMMUNE RESPONSE IN MICE

Julia Wagner, Dorothee Göbl, Natasha Ustyanovsk, Mengyao Xiong, Daniel Hauser, Olga Zhuzhgova, Sandra Hocevar, Betül Taskoparan, Laura Poller, Stefan Datz, **Hanna Engelke**, Youssef Daali, **Thomas Bein**, and Carole Bourquin

- <https://pharmazie.uni-graz.at/de/forschen/pharmazeutische-chemie/molekulare-pharmazie/pharmazeutische-zellbiologie/>
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In this collaborative study, the group synthesized mesoporous silica nanoparticles (MSNs) equipped with a pH-responsive capping system as a carrier for the immunostimulatory drug R848. After careful characterization of their stability and activation properties in cell culture, they assessed their potential for enhancing local immune responses in mice.

The main findings are:

- The pH-responsive avidin cap tightly closes the MSN pores at physiological pH and efficiently opens at low pH to release its cargo.
- MSNs are taken up into the acidic lysosomes of dendritic cells, where they cause strong immune activation.
- In mice, MSNs accumulate in migratory dendritic cells in the draining lymph nodes, where they potently enhance immune activation.
- MSNs significantly improve the pharmacokinetic profile of R848 in mice.

Small molecule drugs such as R848 tend to be rapidly eliminated from the body. This research shows that MSNs drastically prolong the half-life of their cargo while systemic exposure to R848 is kept low. Current literature rarely provides such an in-depth pharmacokinetic profile of a nanoparticle-delivered drug. Furthermore, efficient loading of the hydrophobic drug R848 into nanoparticles and the control of R848 release from the particles has until now represented a challenge. Thanks to the stimuli-responsive cap on the multifunctional MSN system, the group was able to potently activate immune cells

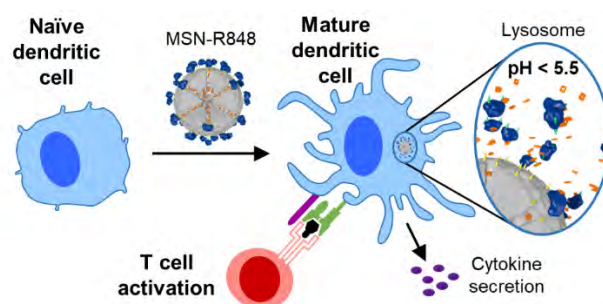


Figure 1. Schematic depiction of the activation of immune cells by means of MSNs serving as stimuli-responsive carriers for the immunostimulant R848.

and at the same time to circumvent a burst release. Overall, they present here a highly versatile nanoparticle platform with a comprehensive characterization of the pharmacokinetics of its cargo.

- **J. Wagner, D. Gossl, N. Ustyanovska, M. Y. Xiong, D. Hauser, O. Zhuzhgova, S. Hocevar, B. Taskoparan, L. Poller, S. Datz, H. Engelke, Y. Daali, T. Bein, C. Bourquin:** *Mesoporous Silica Nanoparticles as pH-Responsive Carrier for the Immune-Activating Drug Resiquimod Enhance the Local Immune Response in Mice*; ACS Nano 15, 4450. 10.1021/acsnano.0c08384 (2021).

ULTRA-THIN PROTECTIVE COATINGS FOR SUSTAINED PHOTOELECTROCHEMICAL WATER OXIDATION WITH MO:BiVO₄

Michael Beetz, Sebastian Häringer, Patrick Elsässer, Jonathan Kampmann, Lena Sauerland, Florian Wolf, Marcella Günther, Anna Fischer, and **Thomas Bein**

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The ever-increasing demand for sustainable forms of energy poses unresolved challenges regarding energy storage and energy conversion. One possible solution is photoelectrochemical water splitting into hydrogen and oxygen with the help of sunlight. Currently, semiconductor materials for water splitting applications require conditions that are still not conducive for large-scale implementation, such as strongly acidic or basic electrolyte media, the use of rare and precious metal catalysts or the need for sacrificial agents to achieve adequate energy conversion rates. In addition, the stability of the photoabsorbers/catalysts remains a challenge. Most of the highly active photocatalysts are subject to severe corrosion after being used for seconds or a few minutes, while longer-term stable materials only provide low photocurrents.

Here, the group presents a successful and scalable protection strategy for the promising photoanode Mo:BiVO₄ that enables record high photocurrents. They examine the impact of ultra-thin conformal and amorphous protective layers such as niobium-doped titania (NTO), tin oxide or aluminum oxide on photocorrosion and dissolution of the photoanode during operating conditions. They demonstrate that

a 2.5 nm thin amorphous NTO layer, applied by atomic layer deposition (ALD), provides an effective way to protect Mo:BiVO₄ photoelectrodes from V⁵⁺ dissolution and corrosion, while preserving the exceptionally high photocurrents of Mo:BiVO₄. Moreover, the group shows that nanoscale Fe:NiO_x employed as co-catalyst enables unprecedented photocurrents of 5.6 mA cm⁻² under environmentally favorable conditions (pH = 7 in NaOH/H₃PO₄ buffer solution without the need for sacrificial agents) at simulated solar AM 1.5G illumination.

This strategy provides a general blueprint for the protection of other water oxidation electrode materials that are prone to corrosion and suffer from dissolution processes. As a result, the independent tunability of the key photoanode components, i.e., photoabsorber, ultrathin protection layer and nanoscale co-catalyst offers a vast parameter space for the design of additional promising photoanodes for the sustainable generation of solar hydrogen.

■ **M. Beetz, S. Häringer, P. Elsässer, J. Kampmann, L. Sauerland, F. Wolf, M. Günther, A. Fischer, T. Bein:** *Ultra-Thin Protective Coatings for Sustained Photoelectrochemical Water Oxidation with Mo:BiVO₄*; *Advanced Functional Materials* 31, 2011210. 10.1002/adfm.202011210 (2021.)

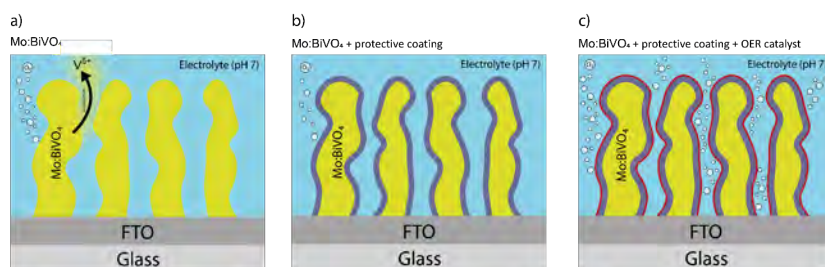


Figure 1. Schemes of Mo:BiVO₄-based photoanodes under operating conditions showing the protection strategy for enhanced durability and performance. (a) Pure Mo:BiVO₄ suffers from corrosion during oxygen evolution by leaching vanadium(V) ions into the electrolyte. (b) A thin protective coating prevents the dissolution of vanadium(V) ions in the electrolyte at reduced photoelectrochemical activity. (c) An additional OER catalyst on-top of the protection layer enables effective water oxidation at reduced corrosion.

FAST-SWITCHING VIS-IR ELECTROCHROMIC COVALENT ORGANIC FRAMEWORKS

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Covalent organic frameworks (COFs) are an emerging class of highly tunable crystalline, porous organic semiconductors. Their molecular-length-scale porosity offers a unique possibility for interactions between the pores and the semiconducting backbone and to introduce stimuli-responsive behavior such as electrochromism.

Classical electrochromic coatings such as WO_3 suffer from low coloration efficiency and slow switching speed. The group has developed highly efficient and fast-switching electrochromic coatings based on fully organic, porous covalent organic frameworks (COFs). The COFs combine a central thienoisindigo moiety with more electron-rich units while fully retaining their favorable stacking interactions. This donor-acceptor-donor electronic setup promotes intramolecular charge transfer, leading to strong light absorption across the visible and near IR regions and an increased sensitivity of the absorption spectra towards electrochemical oxidation. The Vis-NIR absorption bands present in the neutral state shift significantly upon electrochemical oxidation. Fully reversible absorption changes by close to 3 optical densities (OD) can be triggered at low operating voltages and low charge per unit area. The champion material reaches an electrochromic coloration efficiency of $858 \text{ cm}^2 \text{ C}^{-1}$ at 880 nm and retains >95% of its electrochromic response over 100 oxidation/reduction cycles. Furthermore, the electrochromic switching is extremely fast with response times below 0.4 s for the oxidation and around 0.2 s for the reduction, outperforming previous COFs by at least an order of magnitude and rendering these materials some of the fastest-switching frameworks to date. This combination of high coloration efficiency and very fast switching reveals intriguing opportunities

for applications of porous organic electrochromic materials.

■ **D. Bessinger, K. Muggli, M. Beetz, F. Auras, T. Bein:** *Fast-Switching Vis-IR Electrochromic Covalent Organic Frameworks*; *Journal of the American Chemical Society* 143, 7351. 10.1021/jacs.0c12392 (2021).

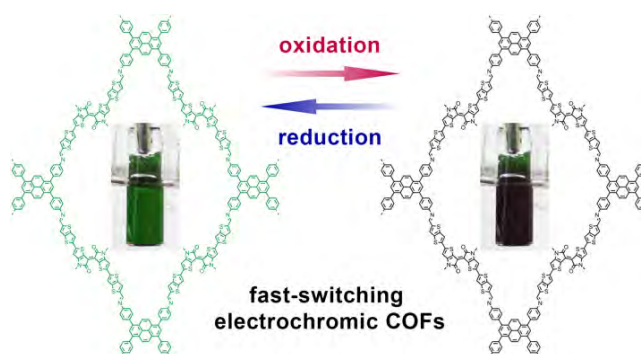


Figure 1. Fragment of the thienoisindigo-based two-dimensional COF that rapidly changes color upon electrochemical oxidation (photographs shown as insets).

STRUCTURED SEQUENCES EMERGE FROM RANDOM POOL WHEN REPLICATED BY TEMPLATED LIGATION

Patrick Kudella, Alexei V. Tkachenko, Annalena Salditt, Sergei Maslov, and Dieter Braun

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The structure of life emerged from randomness. This is attributed to selection by molecular Darwinian evolution. This study found that random templated ligation led to the simultaneous elongation and sequence selection of oligomers. Product strands showed highly structured sequence motifs which inhibited self-folding and built self-templating reaction networks. By the reduction of the sequence space, the kinetics of duplex formation increased and led to a faster replication through the ligation process.

The Eigen theory of replication states, for sequences that are copied one base at a time, that the replication fidelity has to surpass an error threshold to avoid that replicated specific sequences become random because of the incorporated replication errors [M. Eigen, *Naturwissenschaften* 58 (10), 465–523 (1971)]. Here, we showed that linking short oligomers from a random sequence pool in a templated ligation reaction reduced the sequence space of product strands. We started from 12-mer oligonucleotides with two bases in all possible combinations and triggered enzymatic ligation under temperature cycles. Surprisingly, we found the robust creation of long, highly structured sequences with low entropy. At the ligation site, complementary and alternating sequence patterns developed. However, between the ligation sites, we found either an A-rich or a T-rich sequence within a single oligonucleotide. Our modeling suggests that avoidance of hairpins was the likely cause for these two complementary sequence pools.

What emerged was a network of complementary sequences that acted both as templates and substrates of the reaction. This self-selecting ligation reaction could be restarted by only a few majority sequences. The findings showed that replication by random tem-

plated ligation from a random sequence input will lead to a highly structured, long, and nonrandom sequence pool. These findings imply that elementary binding properties of nucleotides can lead to an early selection of sequences even before the onset of Darwinian evolution. This suggests that such a simplification of sequence space could result in faster downstream selection for sequence-based function for the origin of life.

■ P. Kudella, A. Tkachenko, A. Salditt, S. Maslov and D. Braun: *Structured sequences emerge from random pool when replicated by templated ligation*; PNAS doi:10.1073/pnas.2018830118 (2021).

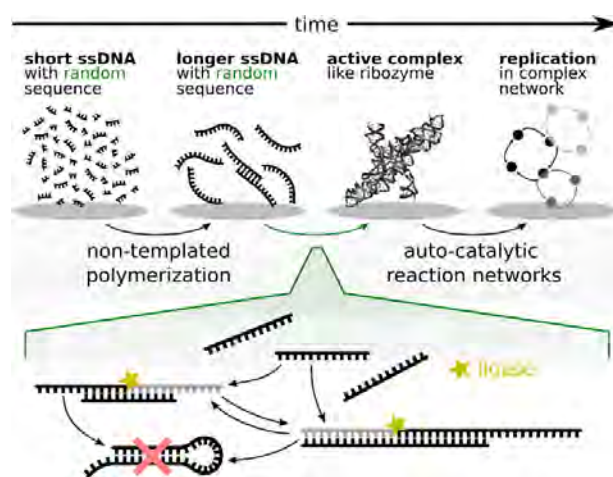


Figure 1. Templated ligation under the non-equilibrium condition of a thermal cycling was found to create structured sequences from randomness. It created networks of complementary strands that increased their replication in a highly cooperative manner, creating by replication significantly decreased sequence structures.

ENGINEERING PLASMONIC AND PHOTONIC MODES FOR PRODUCING SOLAR FUELS

Ludwig Hüttenhofer, Matthias Golibrzuch, Oliver Bienek, Fedja J. Wendisch, Rui Lin, Markus Becherer, Ian D. Sharp, **Stefan A. Maier**, and **Emiliano Cortés**

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The use of plasmonics and photonics to control light and heat close to the thermodynamic limit enables exciting opportunities for nanoscale energy conversion. The efficient harvesting and conversion of photons into photons of a different energy, phonons or energetic charge carriers open up a myriad of opportunities for converting, for example sunlight, into fuels, heat and light. By employing artificially structured materials (metamaterials), hybrid plasmonic colloids, dielectric nanoresonators or engineered metal nanoantennas, my group has shown different approaches for converting energy by controlling, tuning and enhancing light-matter interactions.

One remarkable example is the GaP metasurface photoelectrode for H₂ evolution reaction developed by L. Hüttenhofer, et al. In here, we exploit the light confinement abilities of the dielectric nanoresonators and combine that with the large scale patterning ability of nanoimprint. As such, we create a millimeter-patterned photoelectrode, which enhances the production of H₂ by 6 times compared to a planar GaP film. Furthermore, we measured a 10 times enhancement of the internal quantum efficiency (IQE) of the metasurface compared to a flat film. We attribute the significant IQE enhancement to the near-surface absorption hot spots in the nanoresonators created by the engineered photonic states. These hot spots facilitate highly efficient and near-surface generation of electron-hole pairs, thereby reducing their recombination probability during migration on the—now shorter—path to the solid/liquid interface compared with the continuous film counterpart.

■ **L. Hüttenhofer, M. Golibrzuch, O. Bienek, F. J. Wendisch, R. Lin, M. Becherer, I. D. Sharp, S. A. Maier, E. Cortés:** *Metasurface Photoelectrodes for*

Enhanced Solar Fuel Generation; *Advanced Energy Materials* 46 (11), 2102877 (2021).

D. Glass, R. Quesada-Cabrera, S. Bardey, P. Promdet, R. Sapienza, V. Keller, S. A. Maier, V. Caps, I. P. Parkin, E. Cortés: *Probing the Role of Atomic Defects in Photocatalytic Systems through Photoinduced Enhanced Raman Scattering;* *ACS Energy Letters* 6 (12), 4273-4281 (2021).

P. H.C. Camargo and E. Cortés: *Plasmonic Catalysis: From Fundamentals to Applications;* (Editors), 352 pages, ISBN 3527826963, John Wiley & Sons (2021).

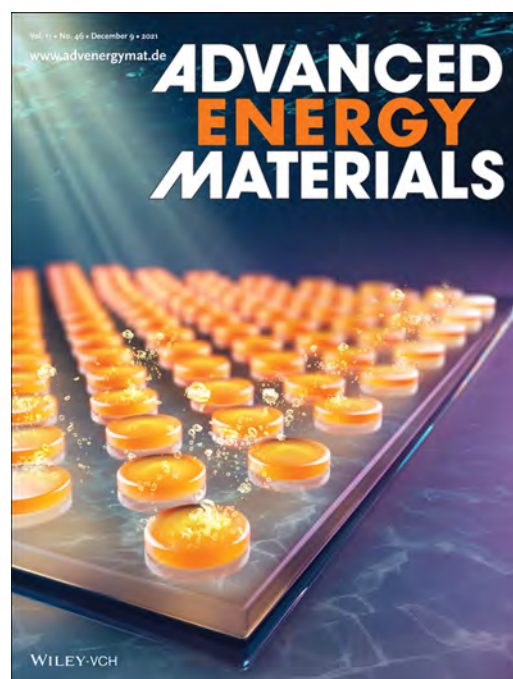


Figure 1. Cover image in *Adv. Energy Mat.* for GaP metasurface photoelectrodes for H₂ generation.

PLASMONIC CATALYSIS, FROM FUNDAMENTALS TO APPLICATIONS

Pedro H. C. Camargo and **Emiliano Cortes** (editors)

■ <https://www.hybridplasmonics.org>

This book delivers a thorough treatment of plasmonic catalysis, from its theoretical foundations to myriad applications in industry and academia. It constitutes the first book in the field and has contributions from worldwide leaders, including Naomi Halas, Peter Nordlander, Pedro Camargo, Emiliano Cortés, Sasha Govorov, Jennifer Dionne, Sebastian Schlücker, Audrey Moores, Prashant Jain, Hiroaki Misawa, Jie Liu, Henry O. Everitt, Hiromi Yamashita, Dong Ha Kim, Wei David Wei and Suljo Linic, among many others.

The book characterizes plasmonic catalytic systems and describes their properties, tackling the integration of conventional and new methods able to unravel the optical, electronic, and chemical properties of these systems. It also describes the fundamentals of controlled synthesis of metal nanoparticles relevant to plasmonic catalysis, as well as practical examples thereof. Readers will also benefit from the inclusion of:

- A thorough introduction to plasmonic catalysis, a theory of plasmons for catalysis and mechanisms, as well as optical properties of plasmonic-catalytic nanostructures;
- An exploration of the synthesis of plasmonic nanoparticles for photo and electro catalysis;
- Plasmonic catalysis towards oxidation reactions and hydrogenation reactions;
- Discussions of plasmonic catalysis for multi-electron processes, artificial photosynthesis and N_2 fixation.
- Mechanistic studies and interfaces of plasmonic structures with semiconductors, metals and molecules.

■ **Pedro H.C. Camargo and Emiliano Cortés (Editors):** *Plasmonic Catalysis: From Fundamentals to Applications*; 352 pages, ISBN 3527826963, John Wiley & Sons (2021).

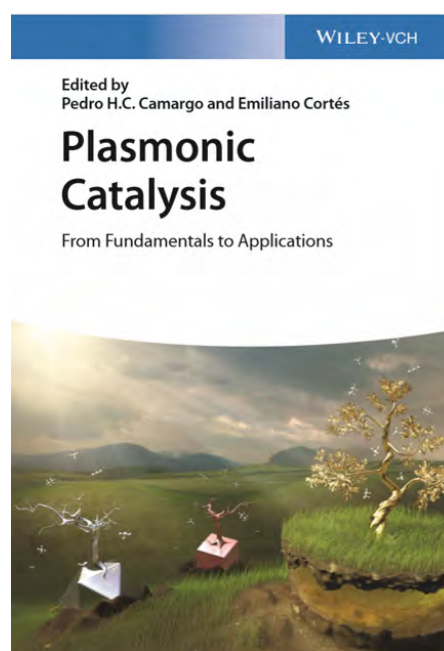


Figure 1. Cover image of the first book on Plasmonic Catalysis, edited by Prof. Camargo (Helsinki University) and Prof. Cortes (LMU).

MULTIPOINT CORRELATION FUNCTIONS: SPECTRAL REPRESENTATION AND NUMERICAL EVALUATION / COMPUTING LOCAL MULTIPOINT CORRELATORS USING THE NUMERICAL RENORMALIZATION GROUP

Fabian B. Kugler, Seung-Sup B. Lee, and **Jan von Delft**

■ https://www.theorie.physik.uni-muenchen.de/17ls_th_solidstate_en

The duo of papers won a CeNS Publication Award 2021 as they provide a breakthrough in quantum many-body physics. Many observables in the experiments of condensed matter and ultracold atoms, such as the conductivity and inelastic scattering spectra, are theoretically described as multipoint correlation functions. However, the analytic structure of multipoint functions has been elusive and their non-perturbative, accurate computations have been intractable. The duo provides answers to these problems. Even before the final publication in Physical Review X (PRX), our work has attracted many experts in the field; currently four international collaborations based on our achievement are ongoing. To our best knowledge, the duo is the first back-to-back publication in PRX by the same team of the authors.

■ **F. B. Kugler, S.-S. B. Lee, and J. von Delft:** *Multipoint Correlation Functions: Spectral Representation and Numerical Evaluation*, Phys. Rev. X 11, 041006 (2021).

■ **S.-S. B. Lee, F. B. Kugler, and J. von Delft:** *Computing Local Multipoint Correlators Using the Numerical Renormalization Group*, Phys. Rev. X 11, 041007 (2021).

OVERCOMING THE CHALLENGES OF FREESTANDING TIN OXIDE-BASED COMPOSITE ANODES TO ACHIEVE HIGH CAPACITY AND INCREASED CYCLING STABILITY

Florian Zoller, Sebastian Häringer, Daniel Böhm, Hannah Illner, Markus Döblinger, Zdenek Sofer, Martin Finsterbusch, **Thomas Bein**, and **Dina Fattakhova-Rohlfing**

■ <https://bein.cup.uni-muenchen.de/>

■ https://www.fz-juelich.de/SharedDocs/Personen/IEK/IEK-1/EN/Fattakhova_Dina.html

Batteries, and lithium-ion batteries in particular, have become an indispensable part of everyday life. The rapid development of new portable electronic devices, electromobility and large-scale energy storage requires batteries with maximum capacity, advanced rate capability and durable cycling performance. Increasing the overall energy density and rate performance of the batteries can be achieved by using materials with an advanced charge storage chemistry and higher theoretical capacities, but also by optimizing the overall electrode architecture and reducing the amount of electrochemically inactive material. In a joint research project between Forschungszentrum Jülich (D. Fattakhova-Rohlfing) and LMU (T. Bein), we have developed a strategy to obtain novel, freestanding antimony-doped tin oxide electrodes with energy density, rate, and cycling performance several times higher than conventional electrodes. Tin oxide is an intensively explored alternative to the currently used graphite active material, as it offers up to 5 times the storage capacity. However, the practically achieved values are much lower due to its poor conductivity and electrochemical

degradation caused by large volume changes. An approach developed by our groups mitigates these drawbacks via nanoscaling to shorten the diffusion paths, doping to increase the electrical conductivity, hybridizing with a conducting carbon matrix to improve electrode conductivity and minimize stresses caused by volume expansion, and finally fabricating freestanding electrodes to further increase energy density on the cell level. With insights into structural optimization, composition and applicable synthesis techniques, our work contributes to the development of future high-performance battery active materials sought by industry and required for a successful transition of the mobility and energy sector towards their electrification.

■ **F. Zoller, S. Häringer, D. Böhm, H. Illner, M. Döblinger, Z. Sofer, M. Finsterbusch, T. Bein, D. Fattakhova-Rohlfing:** *Overcoming the Challenges of Freestanding Tin Oxide-Based Composite Anodes to Achieve High Capacity and Increased Cycling Stability*; *Adv. Funct. Mater.*, doi.org/10.1002/adfm.202106373 (2021).

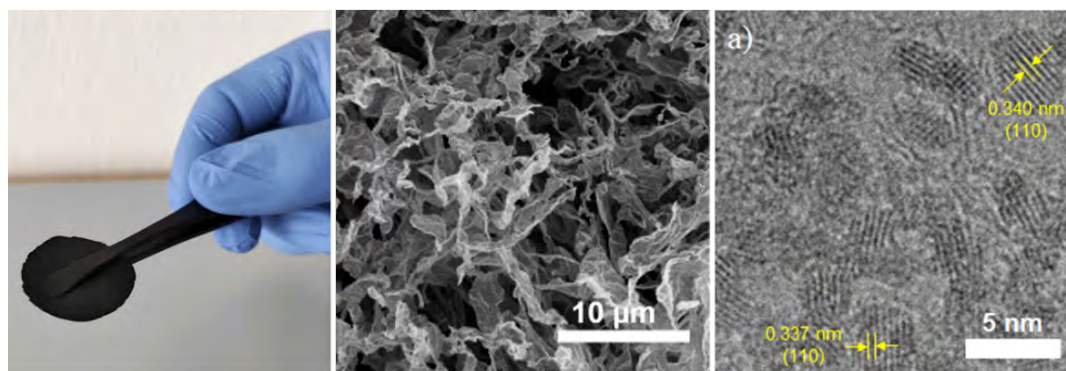


Figure 1. Free-standing antimony-doped tin oxide (ATO) electrodes at different length scales: photo of the whole electrode (left), SEM image of the porous graphene backbone decorated with ATO nanoparticles (middle) and TEM image of the ATO nanoparticles attached to graphene (right)

NANOSCALE FASL ORGANIZATION ON DNA ORIGAMI TO DECIPHER APOPTOSIS SIGNAL ACTIVATION IN CELLS

Ricarda M. L. Berger, Johann M. Weck, Simon M. Kempe, Oliver Hill, **Tim Liedl**, **Joachim O. Rädler**, Cornelia Monzel, and **Amelie Heuer-Jungemann**

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

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

Cell signalling is initiated by characteristic protein patterns in the plasma membrane, but tools to decipher their molecular organization and activation are lacking. Tools enabling acute control of such complex formation or its inhibition with effects on the signalling pathway are of primary interest in fundamental cell biology or nanomedicine. Among the signalling complexes which present themselves as supramolecular assemblies, members of the tumor necrosis factor (TNF) super family are extensively studied and models of their multimerization and cluster formation have been proposed. Within this family, trimeric Fas ligand (FasL) plays a pivotal role in cell decision making towards proliferation or apoptosis. FasL is mainly expressed by cytotoxic T cells and eliminates cancer cells by FasL-mediated

apoptosis. Present models of Fas signal initiation suggest that Fas receptors (FasR) may pre-arrange in trimers assembling into hexameric patterns on the membrane. Upon binding of trimeric FasL, they may further arrange in hexameric supramolecular structures with ~ 10 nm intermolecular spacing in order to induce signal initiation. In a very fruitful collaboration between the CeNS groups of A. Heuer-Jungemann, T. Liedl and J. Rädler together with C. Monzel from the HHU Düsseldorf, we probed this architecture by arranging FasL in hexameric geometries on DNA origami platforms. These nanoagents act as signalling platforms inducing fastest time-to-death kinetics for hexagonal FasL arrangements with 10 nm inter-molecular spacing. Compared to naturally occurring soluble FasL, this trigger is faster and

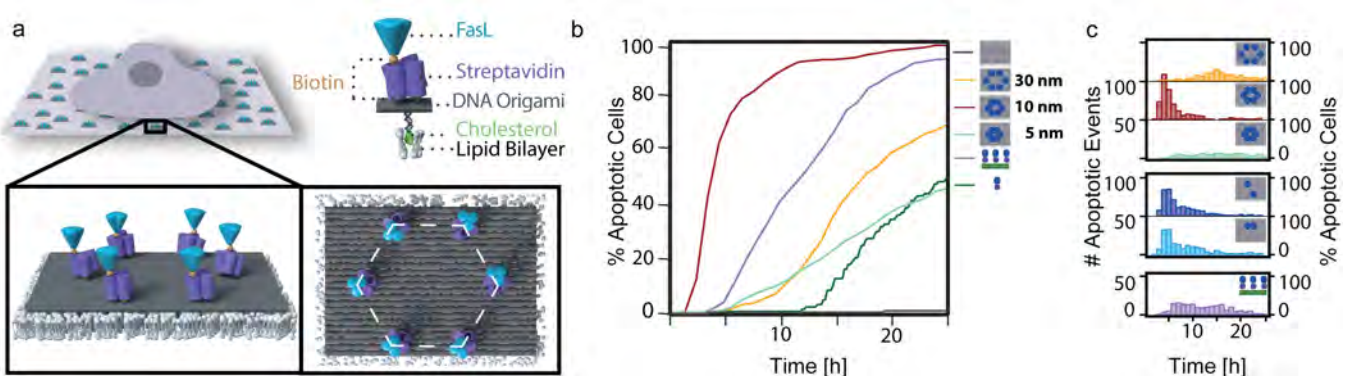


Figure 1. (a) Schematic illustration of a cell seeded on DNA origami grafted to a supported lipid membrane. The magnifications show the Streptavidin-Biotin mediated linkage of trimeric Fas ligand to DNA origami. Top view illustrates the hexagonal arrangement indicated by white dashed lines. (b) Percentage of apoptotic cells in population for different FasL-FasL distances arranged on DNA origami platforms and (c) Histogram of time-to-death data, normalized to 200 cells per histogram. FasL induced apoptosis is most efficient for the nanoagent with 10 nm inter-ligand distance (red) compared to 30 (yellow) or 5 nm (light green) inter-ligand distances. FasL-functionalized lipid membranes (lilac) are more efficient at inducing apoptosis than FasL in solution (dark green). Bare DNA origami show no significant apoptosis induction (grey).

100× more efficient. Nanoagents with different spacing, lower FasL number or higher coupling flexibility impeded signalling. Our results confirm the current theoretical models of FasR oligomerization and constitute a valuable result for future nanomedical approaches especially with a view towards cancer therapy and the development of agents for the treatment of auto-immune diseases. We showed that DNA origami is an excellent tool to define molecular benchmarks in apoptosis signal initiation and

presents a new strategy to drive particular cell responses.

■ **R. M. L. Berger, J. M. Weck, S. M. Kempe, O. Hill, T. Liedl, J. O. Rädler, C. Monzel* and A. Heuer-Jungemann***: *Nanoscale FasL Organization on DNA Origami to Decipher Apoptosis Signal Activation in Cells*; *Small*, doi:10.1002/smll.202101678 (2021).

11

OPEN-CAVITY IN CLOSED-CYCLE CRYOSTAT AS A QUANTUM OPTICS PLATFORM

Samarth Vadia, Johannes Scherzer, Holger Thierschmann, Clemens Schäfermeier, Claudio Dal Savio, Takashi Taniguchi, Kenji Watanabe, David Hunger, **Khaled Karrai**, and **Alexander Högele**

■ www.nano.physik.uni-muenchen.de/nanophotonics

The work demonstrates the operation of an open-cavity in a closed-cycle cryostat as a cryogenic platform for cavity quantum optics with solid-state. The open cavity system consists of a planar mirror supporting solid-state emitters, and a concavely shaped tip of an optical fiber. The fiber micro-mirror and the macroscopic mirror can be moved with respect to each other, thus providing large spatial and spectral tunability. The mitigation of vibrations in the harsh environment of a closed-cycle cryostat is the key result of the collaborative work. With a combination of passive and active vibration reduction techniques, the root mean square cavity length fluctuations were reduced down to less than 100 pm, representing an improvement by more than five orders of magnitude compared to the typical mechanical vibrations induced by a closed-cycle cryo-cooler. The stability achieved enables experiments with cavity quality factors of up to 1 million, providing sufficient light-matter coupling for the strong coupling regime as demonstrated by the formation of exciton polaritons in semiconducting monolayer of WSe_2 .

■ **S. Vadia, J. Scherzer, H. Thierschmann, C. Schäfermeier, C. Dal Savio, T. Taniguchi, K. Watanabe, D. Hunger, K. Karrai, and A. Högele**; *Open-Cavity in Closed-Cycle Cryostat as a Quantum Optics Platform*; *PRX Quantum* 2, 040318 (2021).

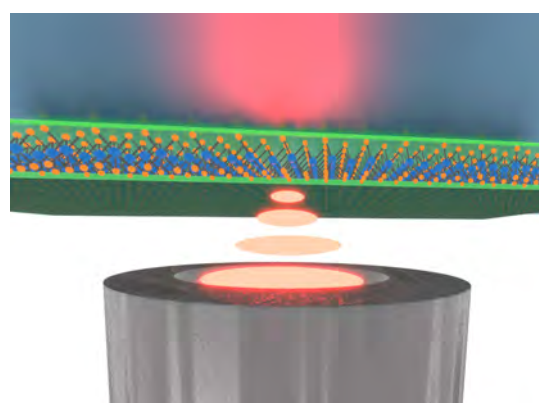


Figure 1. Open cavity formed by a microscopic fiber-mirror and a macroscopic planar mirror with a monolayer semiconductor WSe_2 , composed of W and Se atoms (indicated by blue and orange spheres). Using passive damping technology, strong light-matter coupling between the cavity photons and semiconductor excitons was achieved in the harsh vibrational environment of a closed-cycle cryostat.

SUPERRESOLUTION INFRARED NEAR-FIELD MICROSCOPY OF LIVING CELLS

Korbinian Kaltenecker, Thorsten Gözl, Enrico Bau, and **Fritz Keilmann**■ https://www.softmatter.physik.lmu.de/personen/former_members/fritz-keilmann1/nanoscopy_lab

Near-field microscopy (s-SNOM) is applied to characterize living cells, at long wavelengths from 5 to 10 μm . This is for the first time that infrared nano-imaging and "fingerprint" nano-spectroscopy on cells are realized in the presence of water. Key to this achievement is the physical separation between sample and observation spaces by a nano-membrane.

The s-SNOM (from CeNS spin-off neaspec, now attocube) uses backscattering from a metal AFM tip which scans the ultrathin (10 nm), flat SiN membrane from above (Fig. 1a), while water-dispersed nano-objects adhere on the membrane's downside. The tip-confined near-field (white patch) penetrates the membrane without loss and maps a living cell's local infrared image (Fig. 1b), at <150 nm resolution. When operated with broad-band infrared illumination the recorded (nano-FTIR) spectrum exhibits characteristic molecular vibration bands which enable mapping the chemical composition, i.e.,

quantifying the cell's local abundances of protein, lipid, DNA and water. Applications in biology and medicine could be in areas such as cell migration and cell differentiation, or for researching protein aggregation in neurodegenerative diseases.

Surprisingly, the s-SNOM further reveals a highly structured mechanical AFM image (Fig. 1c) that partly correlates with the infrared image. Obviously the cell deforms the membrane locally. While the mechanism underlying this attraction is to be investigated, the practical significance for cell characterization is that it provides a map of local adhesion forces, apart from holding cells in place for prolonged observation.

The liquid cell construction is leak-tight and enables continuously following a living cell's morphological and chemical development. The robust setup should enable the nano-chemical analysis of any liquid-based, dynamic process.

Besides, we show in theory and experiment that the infrared near field penetrates about 100 nm deep below the SiN membrane which thus determines the depth range that the s-SNOM probes into cellular organisms.

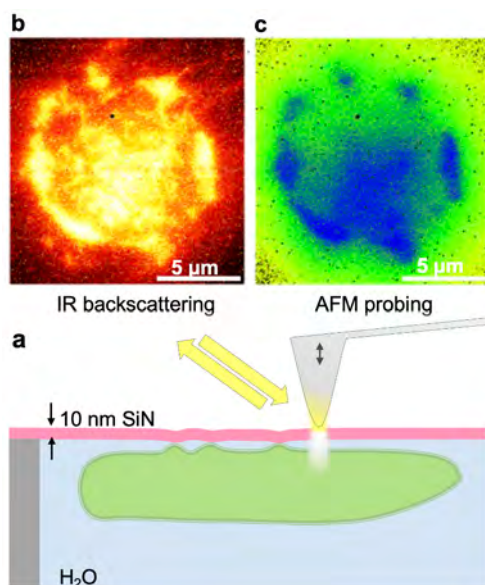


Figure 1. Sketch (a) and results (b,c) of in-vivo imaging a lung cancer cell of type A549, prepared by simply drop-casting a liquid culture onto the 10-nm thin SiN membrane where cells adhere. The infrared backscattering image (b) maps the cell's morphology in <150 -nm detail, whereas the simultaneous AFM probing (c) clearly exhibits a correlated mechanical phase contrast image, interpreted as the cell's adhesion footprint.

■ **K. J. Kaltenecker, T. Gözl, E. Bau, F. Keilmann:** *Infrared-spectroscopic, dynamic near-field microscopy of living cells and nanoparticles in water.* Scientific Reports 11, 21860 doi.org/10.1038/s41598-021-01425-w (2021).

ON-SURFACE PHOTOPOLYMERIZATION OF TWO-DIMENSIONAL POLYMERS ORDERED ON THE MESOSCALE

Markus Lackinger and Wolfgang Heckl

■ <https://www.edu.sot.tum.de/en/wisskom>

2D polymers are a novel class of low dimensional organic materials with projected applications in separation, sensorics, catalysis and molecular electronics. Current challenges concern the rational bottom up synthesis as well as molecularly resolved structural characterization. Here, we employ solid surfaces to template the targeted 2D topology. The synthetic route comprises the topochemical photopolymerization of fluorinated anthracene-triptrycene (fantrip) monomers. The underlying protocol is two-staged: (1) Self-assembly of the monomers into a photopolymerizable monolayer structure, where the photoactive anthracene moieties are face-to-face stacked; (2) cross-linking of the self-assembled monolayer into a covalent 2D polymer by [4+4] photocycloadditions between the aligned anthracene blades. This approach crucially depends on achieving the reactive packing, whereby the underlying surface plays a decisive role for self-assembly. We used graphite, but additional passivation with an alkane monolayer was necessary to weaken molecule-surface interactions. As a result, the desired monolayer with enhanced molecule-molecule interactions became thermodynamically preferred. Scan-

ning Tunneling Microscopy (STM) has proven to be the ideal analytical tool for monitoring the progression of the polymerization with the ultimate single-linkage resolution. The [4+4] cycloadditions induce a sizable increase of the HOMO-LUMO gap, which translates into an unambiguous change of STM contrast. Successful photopolymerization could be corroborated by complementary local IR spectroscopy and mass spectrometry. The possibility to identify individual covalent linkages by STM facilitated studies of the polymerization progression and allowed to assess the temperature dependence of polymerization rates, where an increase with temperature indicated a small energy barrier in the photoexcited state. Future research is directed towards the synthesis of 2D polymers with macroscopic extensions.

■ **L. Grossmann, B.T. King, S. Reichlmaier, N. Hartmann, J. Rosen, W.M. Heckl, J. Björk, M. Lackinger:** *On-surface photopolymerization of two-dimensional polymers ordered on the mesoscale;* Nature Chemistry, 10.1038/s41557-021-00709-y (2021).

M. Lackinger and A.D. Schlüter: *The Current Understanding of how 2D Polymers Grow Photochemically;* European Journal of Organic Chemistry, 10.1002/ejoc.202101006 (2021).

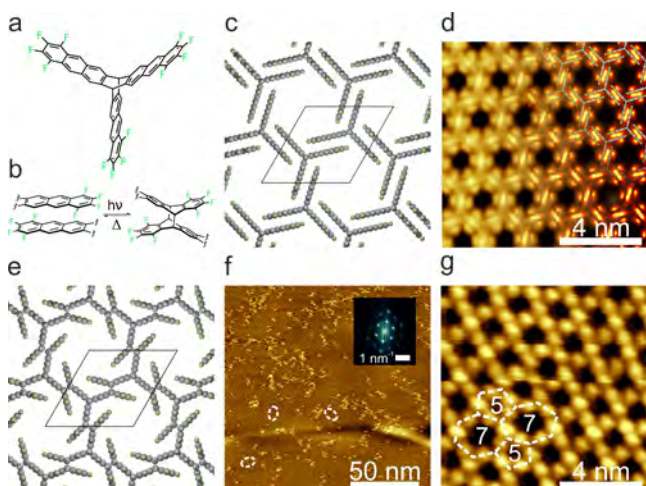


Figure 1. 2D polymer synthesis by photopolymerization. (a) fantrip monomer; (b) reaction scheme; (c) model (top view) and (d) STM image as well as corresponding simulation (right hand side) of the initial supramolecular structure; (e) model and (f), (g) STM images of the resulting 2D polymer; (g) shows the structure of a typical defect that is isostructural to the well-known Stone-Wales defect in graphene.

COMPARATIVE ANALYSIS OF THE COORDINATED MOTION OF HSP70S FROM DIFFERENT ORGANELLES OBSERVED BY SINGLE-MOLECULE THREE-COLOR FRET

Lena Voith von Voithenberg, Andes Barth, Vanessa Trauschke, Benjamin Demarco, Swati Tyagi, Christine Koehler, Edward A. Lemke, and **Don C. Lamb**

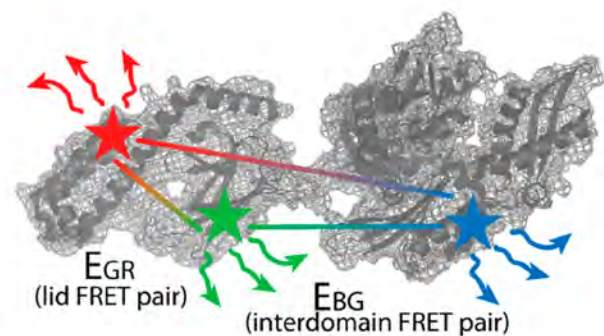
■ <https://www.cup.uni-muenchen.de/pc/lamb>

Over the last few years, my group has been working on ways to quantitatively analyze three-color Förster Resonance Energy Transfer experiments. The ability to measure three-colors and hence three-distances simultaneously on the same molecule opens up new possibilities for biomolecular studies. The new dimensions added with the third color makes the analysis more sensitive to the conformation of the protein and allows the detection of subspecies that would be overlooked in a one-dimensional FRET analysis. It also makes it possible to investigate coordinated conformational changes within a single molecule, allowing unprecedented studies of allosteric effects in biomolecules. Based on our three-color photon-distribution-analysis (3cPDA) published in 2019, we present in this publication the first application of 3cPDA, which we used to investigate the function of heat shock proteins 70s (Hsp70s). From this well-conserved family of important molecular chaperones, we compared three Hsp70s from three different organelles. DnaK (from the cytosol of *E. coli*), Ssc1 (from the mitochondria of yeast) and BiP (from the endoplasmic reticulum from mouse cells). In this paper, the key findings are:

- 1) Discovery of new intermediate conformations indicating the conformational flexibility of the Hsp70 conformational landscape
- 2) That BiP demonstrates a high correlation between conformations of its two domains where as DnaK and Ssc1 showed uncoupled behavior. This illustrates of the evolutionary diversity of the Hsp70s where various cellular compartments adopt the functionality of the Hsp70s for performing different tasks.
- 3) The various Hsp70s have different sensitivities to different nucleotide analogs, suggesting variability in the recognition mechanism of the nucleotide-binding domain.

- 4) A first demonstration of the power and applicability of 3cPDA for investigating coordinated motions within a single biomolecule.

■ **L. Voith von Voithenberg, A. Barth, V. Trauschke, B. Demarco, S. Tyagi, C. Koehler, E. A. Lemke, and D. C. Lamb:** *Comparative analysis of the coordinated motion of Hsp70s from different organelles observed by single-molecule three-color FRET*; PNAS 118 (2021).



DOUBLE-TO SINGLE-STRAND TRANSITION INDUCES FORCES AND MOTION IN DNA ORIGAMI NANOSTRUCTURES

Fatih N. Gür, Susanne Kempter, Florian Schueder, Christoph Sikeler, Maximilian J. Urban, **Ralf Jungmann**, Philipp C. Nickels, and **Tim Liedl**

- https://www.softmatter.physik.uni-muenchen.de/liedl_group
- <https://www.biochem.mpg.de/jungmann>

DNA nanotechnology has transformed our understanding of self-assembly processes and DNA origami in particular has opened up new routes for building complex materials and devices. Arguably one of the most intricate fields of applications is the design and implementation of self-assembled nanoscale machines and motors. Here we introduce the concept of a defined pulling mechanism making use of the entropic spring behaviour of single-stranded DNA. We show controlled and reversible motion of two 40 nm long arms that are pulled together by a stretch of single-stranded DNA, resembling the arms of a jumping jack. The opening and closing of the arms is monitored with a variety of techniques including super-resolution microscopy and plasmon resonance spectroscopy. For the latter

we attached 50 nm “large” gold nanoparticles as a cargo, demonstrating the robustness of our approach.

In summary, the pre-designed stress inside DNA objects can be employed to provoke large controlled conformational changes. This could be further developed to control mechanical signal transduction over long distances in response to trigger events such as mRNA detection or enzymatic activity.

■ **F. N. Gür, S. Kempter, F. Schueder, C. Sikeler, M. J. Urban, R. Jungmann, T. Liedl:** *Double-to Single-Strand Transition Induces Forces and Motion in DNA Origami Nanostructures*; *Advanced Materials* 33 (37), 2101986 (2021).

VISCOELASTIC BEHAVIOR OF CHEMICALLY FUELED SUPRAMOLECULAR HYDROGELS UNDER LOAD AND INFLUENCE OF REACTION SIDE PRODUCTS

Martin Kretschmer, Benjamin Winkeljann, Brigitte A.K. Kriebisch, Job Boekhoven, and **Oliver Lieleg**

■ <https://www.mae.ed.tum.de/en/bme>

About ten years ago, chemically fueled systems have emerged as a new class of synthetic materials with tunable properties. Yet, applications of these materials are still scarce. In part, this is due to an incomplete characterization of the viscoelastic properties of those materials, which has – so far – mostly been limited to assessing their linear response under shear load. Here, we fill some of these gaps by comparing the viscoelastic behavior of two different, carbodiimide fueled Fmoc-peptide systems. We find that both, the linear and non-linear response of the hydrogels formed by those Fmoc-peptides depends on the amount of fuel driving the self-assembly process – but hardly on the direction of force application. In addition, we identify the concentration of accumulated waste products as a novel, so far

neglected parameter that crucially affects the behavior of such chemically fueled hydrogels. With the mechanistic insights gained here, it should be possible to engineer a new generation of dynamic hydrogels with finely tunable material properties that can be tailored precisely for such applications, where they are challenged by mechanical forces.

■ **M. Kretschmer, B. Winkeljann, B.A.K. Kriebisch, J. Boekhoven, and O. Lieleg:**

Viscoelastic behavior of chemically fueled supramolecular hydrogels under load and influence of reaction side products; Communications Materials, 2, 97 doi.org/10.1038/s43246-021-00202-6 (2021).

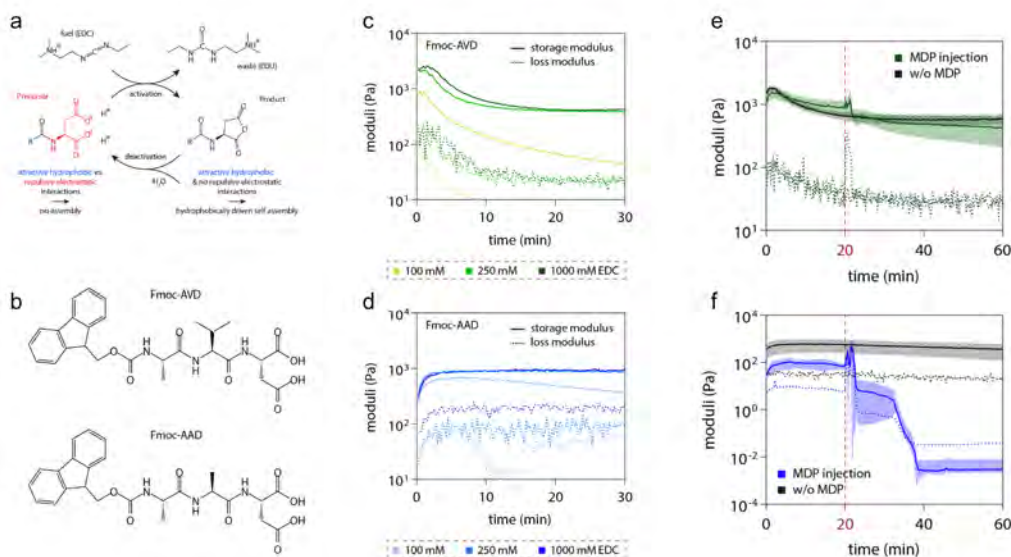


Figure 1. Transient hydrogels are assembled from Fmoc-peptide conjugates which – driven by a chemical reaction (a) are converted from a precursor state into a self-assembling state. The chemical structures of the two peptide variants studied here, Fmoc-AVD and Fmoc-AAD, are depicted in (b). By tuning the fuel concentration driving the chemical background reaction, the life-time of the self-assembled hydrogels can be tuned (c, d). In addition, for one of the peptide variants (Fmoc-AAD, f), controlled disassembly of the hydrogel is possible by adding a molecule (MPD) that mimics the waste product of the chemical reaction cycle (EDU). In contrast, Fmoc-AVD hydrogels are more resistant and withstand this molecular interference step.

HIGH-THROUGHPUT AFM IMAGING AND ANALYSIS REVEALS THE CONFORMATIONAL LANDSCAPE OF NUCLEOSOMES

Sebastian F. Konrad, Willem Vanderlinden, and **Jan Lipfert**

■ <https://www.molecularbiophysics.physik.lmu.de>

In each of our cells, the 2 m-long DNA genome needs to be packed into a ~ 10 μm -sized nucleus, yet remain accessible for read out and replication. This feat is achieved through hierarchical interactions with protein and organization into chromatin. Nucleosomes, which consist of ~ 150 base pairs of DNA wrapped around a core of histone proteins, are the fundamental units of chromatin. We have developed a high-throughput pipeline to image nucleosomes using atomic force microscope imaging to reveal the conformational ensemble of nucleosome structures and investigates how they are altered by epigenetic modifications, i.e. by chemical marks or “annotations” on the histone proteins that are known to play a major role in regulating the read out of our genome. Using a state-of-the-art AFM and optimized sample preparation and imaging protocols, we obtain > 1000 individual nucleosome images in a single field of view. Analyzing such enormous data sets by hand would be tedious and prone to user bias. We have, therefore, created an analysis pipeline using tools from machine learning and image processing to assign and analyse the molecular structures in a fully automated fashion. Our results reveal how nucleosomes can “breathe”, i.e. how the DNA can dynamically fluctuate and unwrap from the histone core. We find that unwrapping occurs in steps of 5 base pairs and can indeed be strongly affected by epigenetic marks.

■ **S. F. Konrad, W. Vanderlinden, W. Frederickx W, T. Brouns, B. H. Menze, S. De Feyter, J. Lipfert:** *High-throughput AFM analysis reveals unwrapping pathways of H3 and CENP-A nucleosomes;* *Nanoscale* 13(10):5435-5447, doi: 10.1039/d0nr08564b (2021).

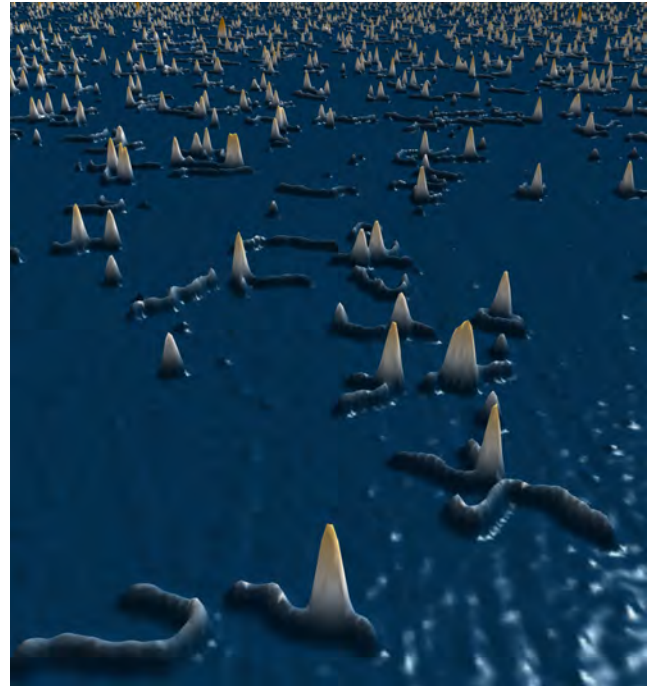


Figure 1. 3D rendering of an AFM height image of nucleosomes co-deposited with bare DNA.

S. F. Konrad, W. Vanderlinden, J. Lipfert: *A High-throughput Pipeline to Determine DNA and Nucleosome Conformations by AFM Imaging.* *Bio Protoc* 11(19):e4180, doi: 10.21769/BioProtoc.4180. (2021).

AN ELECTRICALLY CONDUCTING THREE-DIMENSIONAL IRON-CATECHOLATE POROUS FRAMEWORK

Andre Mähringer, Markus Döblinger, Matthias Hennemann, Christoph Gruber, Dominik Fehn, Patricia I. Scheurle, Pouya Hosseini, Irina Santourian, Alfred Schirmacher, Julian M. Rotter, Gunther Wittstock, Karsten Meyer, Timothy Clark, **Thomas Bein**, and **Dana D. Medina**

■ <https://bein.cup.uni-muenchen.de>

Here, we report the synthesis of a unique cubic metal-organic framework (MOF), the Fe-HHTTP-MOF, comprising hexahydroxytriphenylene (HHTTP) supertetrahedral units and Fe(III) ions, arranged in a diamond topology. The MOF is synthesized under solvothermal conditions, yielding a highly crystalline, deep black powder, with crystallites of 300-500 nm size and tetrahedral morphology. Nitrogen sorption analysis indicates a highly porous material with a surface area exceeding 1400 m² g⁻¹. Furthermore, Fe-HHTTP-MOF shows broadband optical absorption from 475 nm up to 1900 nm with excellent absorption capability of 98.5% of the incoming light over the visible spectral region. Electrical conductivity measurements of pressed pellets reveal a high intrinsic electrical conductivity of up to 10⁻³ S cm⁻¹. Quantum mechanical calculations predict Fe-HHTTP-MOF to be an efficient electron conductor, exhibiting continuous charge-carrier pathways throughout the structure. This report expands the paradigm of intrinsically electroactive MOFs, serving as a solid basis for the development of highly porous, ordered frameworks with enhanced electrical conductivity.

■ **P. I. Scheurle, A. Mähringer, A. Biewald, A. Hartschuh, T. Bein, D. D. Medina***: *MOF-74(M) films obtained through vapor-assisted conversion – impact on crystal orientation and optical properties*; Chem. Mater., 10.1021/acs.chemmater.1c00743 (2021).

L. Frey, J. J. Jarju, L. M. Salonen and D. D. Medina: *Boronic-acid-derived covalent organic frameworks: from synthesis to applications*; New J. Chem., 10.1039/D1NJ01269J (2021).

A. Mähringer, M. Döblinger, M. Hennemann, C. Gruber, D. Fehn, P. I. Scheurle, P. Hosseini, I. Santourian, A. Schirmacher, J. M. Rotter, G. Wittstock, K. Meyer, T. Clark, T. Bein, and D. D. Medina: *An electrically conducting three-dimensional iron-catecholate porous framework*; Angew. Chem. Int. Ed, 10.1002/ange.202102670 (2021).

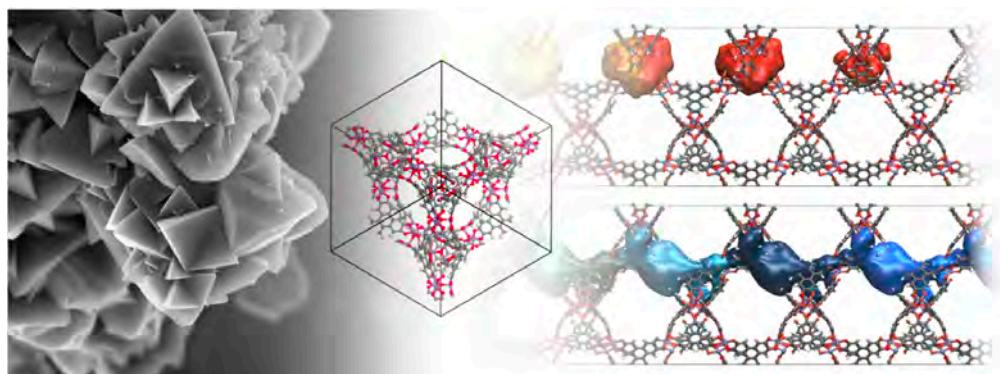


Figure 1. A novel electrically conducting iron HHTTP metal organic frameworks

ENERGY EFFICIENT ULTRAHIGH-FLUX SEPARATION OF OILY POLLUTANTS FROM WATER WITH SUPERHYDROPHILIC NANOSCALE METAL-ORGANIC FRAMEWORK ARCHITECTURES

Andre Mähringer, Matthias Hennemann, Timothy Clark, **Thomas Bein**, and **Dana D. Medina**

■ <https://bein.cup.uni-muenchen.de>

The rising demand for clean water for a growing and increasingly urban global population is one of the most urgent issues of our time. Particularly, the increasing generation of wastewater by cities and industrial sources requires the development of novel platforms for separating contaminants such as oils. Here, we introduce the synthesis of a unique nanoscale architecture of pillar-like Co-CAT-1 metal-organic framework (MOF) crystallites on gold-coated woven stainless steel meshes with large, 50 μm apertures. These nanostructured mesh surfaces feature superhydrophilic and underwater superoleophobic wetting properties, allowing for gravity-driven, highly efficient oil-water separation featuring water fluxes of up to nearly one million $\text{L m}^{-2} \text{h}^{-1}$. Water physisorption experiments reveal the hydrophilic nature of Co-CAT-1 with a total water vapor uptake at room temperature of $470 \text{ cm}^3 \text{ g}^{-1}$. Furthermore, semiempirical molecular orbital calculations shed light on water affinity of the inner and outer pore surfaces. The MOF-based membranes enable high separation efficiencies for a number of liquids tested,

including the notorious water pollutant, crude oil, affording chemical oxygen demand (COD) concentrations below 25 mg L^{-1} of the effluent. Our results demonstrate the great impact of suitable nanoscale surface architectures as a means of encoding on-surface extreme wetting properties, yielding energy-efficient water-selective large-aperture membranes. The extremely low resistance to flow and the resulting enormous flux capabilities hold great promise for water cleanup on a massive scale and for the design of practical, low-cost water purification devices that can be operated without external power source and without moving parts.

■ **A. Mähringer, M. Hennemann, T. Clark, T. Bein, D. D. Medina:** *Energy efficient ultrahigh-flux separation of oily pollutants from water with superhydrophilic nanoscale metal-organic framework architectures*; *Angew. Chem. Int. Ed.*, 10.1002/anie.202012428 (2021).

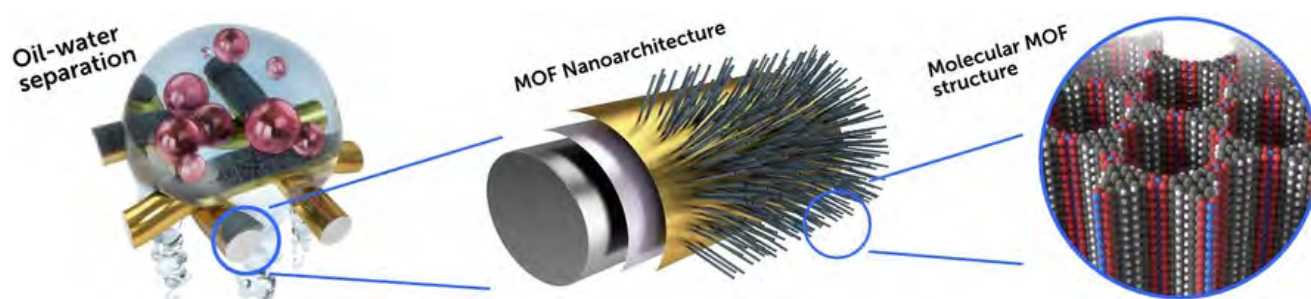


Figure 1. A Schematic illustration of the oil-water separation by the Co-CAT-1@Au@SSM membrane blocking oil flux and allowing only water to pass through the apertures. Cross-sectional visualization of a fabricated Co-CAT-1@Au@SSM string. The Co-Cat-1 crystals are comprised of metal-ions in-plane coordinated by 2,3,6,7,10,11-hexahydroxytriphenylene units forming hexagonally structured 2D layers. Finally, the MOF forms needle-like crystallites on the gold patterns encoding superhydrophilic properties on the mesh.

ULTRAHIGH SPATIAL RESOLUTION TEMPERATURE SENSING WITH SINGLE NANOPARTICLES

Leonardo de Souza Menezes

■ <https://www.hybridplasmonics.org>

Many years ago, it was shown that an Er^{3+} doped special glass could be used as an optical temperature sensor. By exciting Er^{3+} ions in a bulk sample with a CW laser emitting at $1.48 \mu\text{m}$ one can detect fluorescence in the visible (process called frequency upconversion-UC). Particularly, two emissions in the green centered at 525 nm and 550 nm are originated in thermally coupled energy levels, that is, their relative occupation follows Boltzmann's population distribution. Thus, by measuring the relative intensities of these two emissions in the green, one determines the sample's temperature if one knows the energy difference between the energy levels involved in the UC process (easily obtained in linear absorption experiments).

Improvements have been done when one started to investigate these effects in ensembles of nanoparticles (NPs) in conditions of biological interest, like when the NPs are imbedded in certain liquids, as water and glycerol. In a step further there are reports in the direction of understanding the role played by the fact that one uses nanostructured materials. For example, monodisperse (but wide distributed in size) ensembles with average particle sizes of 26 nm and 58 nm have been investigated and clearly showed different thermometer behaviors.

Whenever one deals with ensembles of NPs one measures the average behavior of their components. When working with single NPs, one really sees the behavior of a NP and the role played by NPs with different sizes can be unambiguously understood. Such size effects were already demonstrated and discussed in the literature, but no temperature effects had been investigated.

Using our expertise in the field and the infrastructure developed in our lab., we aim at exploiting temperature effects in UC processes in single rare-earth doped NPs, like Y_2O_3 , NaYF_4 and Gd_2O_3 doped with Er^{3+} , Yb^{3+} and Nd^{3+} due to their potential applications

in real life. The first steps towards this goal have been recently demonstrated by us.

■ **J. A. O. Galindo, A. R. Pessoa, A. M. Amaral, L. F. dos Santos, R. R. Gonçalves, and L. de S. Menezes:** *Influence of the surrounding medium on the luminescence-based thermometric properties of single $\text{Yb}^{3+}/\text{Er}^{3+}$ codoped yttria nanocrystals;* *Nanoscale Advances*, doi 10.1039/D1NA00466B (2021).

I. M. Gonçalves, A. R. Pessoa, C. Hazra, Y. S. Correales, S. J. L. Ribeiro, and L. de S. Menezes: *Phonon-assisted NIR-to-visible upconversion in single NaYF_4 microcrystals doped with Er^{3+} and Yb^{3+} for microthermometry applications: experiment and theory;* *Journal of Luminescence*, doi 10.1016/j.jlumin.2020.117801 (2021).

R. Galvão, L. F. dos Santos, K. de O. Lima, R. R. Gonçalves, and L. de S. Menezes: *Single $\text{Er}^{3+}/\text{Yb}^{3+}$ codoped yttria nanocrystals for temperature sensing: experimental characterization and theoretical modelling;* *The Journal of Physical Chemistry C*, doi 10.1021/acs.jpcc.1c03058 (2021).

R. Galvão, L. F. Santos, R. R. Gonçalves, and L. S. Menezes: *Fluorescence Intensity Ratio-based temperature sensor with single $\text{Nd}^{3+}:\text{Y}_2\text{O}_3$ nanoparticles: Experiment and theoretical modeling;* *Nano Select*, doi 10.1002/nano.202000148 (2021).

K. de O. Lima, L. F. dos Santos, R. Galvão, A. C. Tedesco, L. de S. Menezes, and R. R. Gonçalves: *Single Er^{3+} , $\text{Yb}^{3+}:\text{KGd}_3\text{F}_{10}$ Nanoparticles for Nanothermometry;* *Frontiers in Chemistry*, doi 10.3389/fchem.2021.712659 (2021).

HIGHLY EFFICIENT METHODS FOR THE FORMATION OF THE KOHN-SHAM MATRIX WITHIN HYBRID DENSITY FUNCTIONAL THEORY

Henryk Laqua, Jörg Kussmann, and **Christian Ochsenfeld**

■ <https://www.cup.lmu.de/pc/ochsenfeld>

The efficient quantum-chemical calculation of static and dynamic properties of molecular systems is essential for gaining deeper insights into chemical processes at the *ab-initio* level. Here, the rate determining step is typically the evaluation of the Kohn-Sham Matrix in each iteration of the self-consistent field (SCF) procedure within hybrid density functional theory (DFT) calculations. In order to overcome this computational bottleneck, we developed highly efficient methods in our group.

In particular, the evaluation of the Coulomb [1], the exact-exchange [2], and the semilocal exchange-correlation (sl-XC) matrix [1] are usually the computational bottlenecks. By employing the resolution-of-the-identity Coulomb (RI-J) approximation and seminumerical integration and exploiting the superior compute performance of graphics processing units (GPUs), we were able to accelerate hybrid-DFT calculations by over two orders of magnitude.

In this way, *in silico* studies on much larger molecular systems can be conducted at much higher accuracy (larger basis sets, better density functional approximations, thorough sampling of the configurational space) with much lower computational cost than before. This allows for much more detailed studies of complex and dynamic molecular environments by e.g., *ab-initio* molecular dynamics (AIMD) simulations or nonadiabatic molecular dynamics (NAMMD) simulations.

The highly efficient methods developed in our group thus enable the exploration of previously - due to their size and complexity - inaccessible systems with a plethora of possible applications, e.g., explicit solvent effects, protein catalysis, photocatalysis, DNA interactions, supramolecular host-guest complexes, and many more.

■ [1] J. Kussmann, H. Laqua, C. Ochsenfeld: *Highly Efficient Resolution-of-Identity Density Functional Theory Calculations on Central and Graphics Processing Units*; J. Chem. Theory Comput., 10.1021/acs.jctc.0c01252 (2021).

[2] H. Laqua, J. Kussmann, C. Ochsenfeld: *Accelerating seminumerical Fock-exchange calculations using mixed single- and double-precision arithmetic*. J. Chem. Phys., 10.1063/5.0045084 (2021).

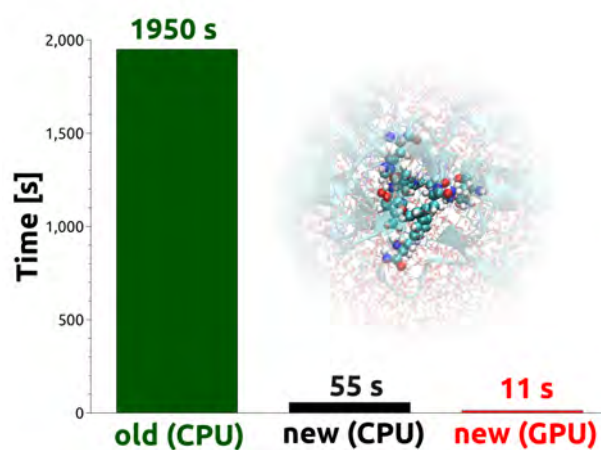


Figure 1. Time for one Kohn-Sham build (B97M-V/def2-TZVPPD) for the active center of Sirtuin-5 (149 QM atoms; see picture) using the old conventional methods (old) and our newly developed methods (new) employing CPUs and GPUs, respectively.

CORRELATIVE, MULTIMODAL MATERIAL CHARACTERIZATION FOR PROBING INTRINSIC AND EXTRINSIC PROPERTIES IN METAL-ORGANIC FRAMEWORK SYSTEMS

Adrian Fuchs, Petra Mannhardt, Patrick Hirschle, Haoze Wang, Irina Zaytseva, Zhe Ji, Omar Yaghi, Stefan Wuttke, and Evelyn Ploetz

■ <https://wuttkescience.com>

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

Reticular materials, especially metal-organic frameworks (MOFs), are employed for a wide range of applications such as energy conversion, carbon and gas storage, sieving, and water harvesting. Due to their high flexibility in synthetic design, the physical and chemical properties of MOFs can easily be tuned, but they also vary considerably with the morphology of individual crystals as well as local structures. It is often unclear how these compositional and structural heterogeneities mutually relate to macroscopic material properties.

Variations occur at different length scales starting from the molecular composition of the MOF in the nanometre regime over long-range ordered crystalline areas on the sub-micrometre scale up to micro- and millimetre-sized MOF particles. To probe their interdependence and access this spatial regime, we developed an *in-situ* methodology that allows for quantifying crystal heterogeneity and its influence beyond the bulk level. We exploit the non-

invasive nature of optical microscopy and spectroscopy for correlative material characterization. The microscope combines space-resolved UV/Vis, fluorescence and Raman spectroscopy with (nonlinear) optical microscopy in a single, confocal system. This correlative approach provides high spatial and spectral resolution for probing the material's response in space and time, which we refer to as multimodal optical spectroscopy and *in-situ* imaging correlation (MOSAIC) analysis.

MOSAIC could highlight for different MOF systems how heterogeneity affects material properties. We could show that the shape has a tremendous influence on the absorption of light by MOF microcrystals, whereas the size did not. This shape-sensitive light absorption could be used for sorting heterogeneous microcrystal compositions. Furthermore, MOSAIC revealed why MOF-801, one of the most promising materials for harvesting water from humid air, does not absorb water evenly – hampering fast cycling of water uptake and release. By correlating the spectral response of four modalities locally, we could identify missing cluster defects as the predominant source for local water clusters.

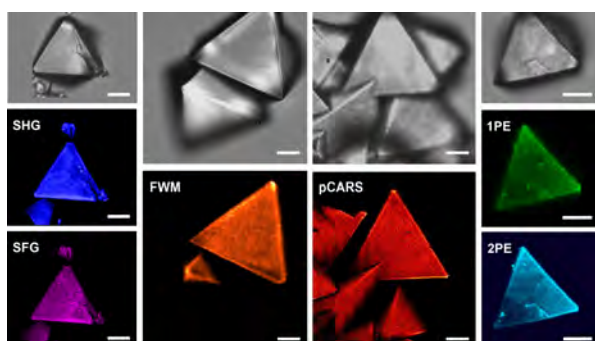


Figure 1. MOSAIC analysis of UiO-67 crystals by spectrally complementary imaging. Unlabeled crystals were studied by brightfield and nonlinear microscopy, based on Second-Harmonic and Sum-Frequency Generation (SHG; SFG), Four-Wave Mixing (FWM) and polarization-sensitive Coherent Anti-Stokes Raman Scattering (pCARS) for probing the surface and inner structure of particles. Confocal fluorescence microscopy was carried out for one- and two-photon excitation (1PE; 2PE) on RBITC-labeled UiO-67 crystals. Scale bars: 10 μm .

■ **A. Fuchs, P. Mannhardt, P. Hirschle, H. Wang, I. Zaytseva, Z. Ji, O.M. Yaghi, S. Wuttke, E. Ploetz:** *Single crystals heterogeneity impacts the intrinsic and extrinsic properties of metal-organic frameworks*; *Advanced Materials*. <https://doi.org/10.1002/adma.202104530> (2021).

TRANSCRIPTION COORDINATES HISTONE AMOUNTS AND GENOME CONTENT

Kora-Lee Claude, Daniela Bureik, Dimitra Chatzitheodoridou, Petia Adarska, Abhyudai Sing, and **Kurt M. Schmoller**

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

Chemical reactions – and as a consequence all biological processes – are governed by the concentrations of the molecules involved. To achieve robust biological outcomes, it is therefore one of the cell's most fundamental tasks to precisely control the amount of its RNA and protein molecules. This is particularly relevant in situations where environmental conditions or cellular programs result in drastic changes of cell morphology and growth rate. Globally, this intricate link between cell size and protein synthesis is thought to be achieved through regulation of the limiting transcriptional and translational machinery. Since larger cells contain a larger amount of limiting machinery, total transcriptional and translational output increases with cell size. Such a simple 'limiting machinery'-mechanism can ensure parallel regulation of a large fraction of proteins while maintaining protein stoichiometry. However, it poses a conundrum for DNA-associated proteins such as histones, whose amount is not proportional to cell size, but instead needs to be coupled to DNA content.

Recently, we showed that even though total protein production increases with cell size, for many DNA-associated proteins amounts are coupled to DNA content and are independent of cell size (Swaffer, *Mol. Cell*, 2021). Using histones as a model, we found that this coupling of proteins to DNA is achieved at the transcript level, and promoters can be sufficient for this regulation. Using genetic manipulations to test predictions we obtained from a mathematical model, we identified a mechanism that allows cells to adjust the proteome as a function of cell size to maintain the stoichiometry of DNA content and histones: while for most genes, transcription is limited by the transcriptional machinery, histone transcription is instead limited by the template, i.e. the gene itself (Claude, *Nat. Comm.*, 2021).

■ **K.-L. Claude, D. Bureik, D. Chatzitheodoridou, P. Adarska, A. Singh, and K. M. Schmoller:** *Transcription coordinates histone amounts and genome content*; *Nature Communications*, 12, 1-17 (2021).

M. P. Swaffer, J. Kim, D. Chandler-Brown, M. Langhinrichs, G.K. Marinov, W. J. Greenleaf, A. Kundaje, K. M. Schmoller, and J. M. Skotheim: *Size-independent mRNA synthesis and chromatin-based partitioning mechanisms generate and maintain constant amounts of protein per cell*, *Molecular Cell*, 81 (23), 4861-4875 (2021).

MASS-SENSITIVE PARTICLE TRACKING TO ELUCIDATE THE MEMBRANE-ASSOCIATED MINDE REACTION CYCLE

Tamara Heermann, Frederik Steiert, Nikolas Hundt, and **Petra Schwill**

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

In spite of their great importance in biology, methods providing access to spontaneous molecular interactions with and on biological membranes have been sparse. The recent advent of mass photometry to quantify mass distributions of unlabeled biomolecules landing on surfaces raised hopes that this approach could be transferred to membranes. Here, by introducing a new interferometric scattering (iSCAT) image processing and analysis strategy adapted to diffusing particles, we enable mass-sensitive particle tracking (MSPT) of single unlabeled biomolecules on a supported lipid bilayer. We applied this approach to the highly nonlinear reaction cycles underlying MinDE protein self-organiza-

tion. MSPT allowed us to determine the stoichiometry and turnover of individual membrane-bound MinD/MinDE protein complexes and to quantify their size-dependent diffusion. This study demonstrates the potential of MSPT to enhance our quantitative understanding of membrane-associated biological systems.

■ **T. Heermann***, **F. Steiert***, **B. Ramm**, **N. Hundt**, **N.**, and **P. Schwill** (* contributed equally): *Mass-sensitive particle tracking to elucidate the membrane-associated MinDE reaction cycle*; *Nat. Methods* 18(10):1239-1246. doi: 10.1038/s41592-021-01260-x (2021).

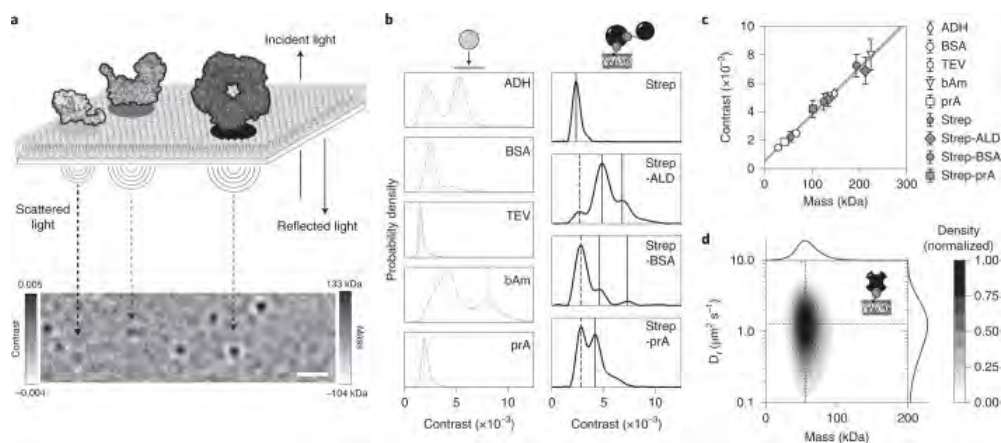


Figure 1. Principle of MSPT. (a) Schematic displaying the iSCAT-based measurement principle of MSPT. Exemplary structures of three aldolase oligomer states are shown in the top panel, and their respective iSCAT images at the bottom. Scale bar, 1 μm . (b) Probability density distributions of standard proteins determined using the conventional mass photometry landing assay (left) or using MSPT (right). All data represent pooled distributions of three independent experiments per condition: alcohol dehydrogenase (ADH) (particle number $n = 9,828$), BSA ($n = 11,408$), TEV protease (TEV) ($n = 1,705$), -amylase (bAm) ($n = 10,043$), protein A (prA) ($n = 12,720$); divalent streptavidin (Strep) ($n = 16,699$ trajectories), divalent streptavidin with biotinylated aldolase (Strep-ALD) ($n = 16,727$ trajectories), divalent streptavidin with biotinylated BSA (Strep-BSA) ($n = 8,842$ trajectories), and divalent streptavidin with biotinylated protein A (Strep-prA) ($n = 22,424$ trajectories). Dashed lines mark peaks not considered for mass calibration (left). Continuous lines represent oligomer states included in the mass calibration. (c) Comparison of the contrast-to-mass calibration for mass photometry and MSPT, derived from peak contrasts in (b) and their assigned sequence masses. Error bars represent the standard error of the peak locations estimated by bootstrapping. (d) Two-dimensional KDE of 1.25 nM tetraivalent streptavidin bound to biotinylated lipids on a SLB ($n = 73,901$ trajectories of three independent replicates; particle density: $0.2 \mu\text{m}^{-2}$). Marginal probability distributions of the molecular mass (top) and the diffusion coefficient (right) are presented.

RETINA ORGANOIDS: WINDOW INTO THE BIOPHYSICS OF NEURONAL SYSTEMS

Katja A. Salbaum, Elijah R. Shelton, and **Friedhelm Serwane**

■ <https://www.serwanelab.org/>

With a kind of magnetism, the human retina draws the eye of neuroscientist and physicist alike. It is attractive as a self-organizing system, which forms as a part of the central nervous system via biochemical and mechanical cues. The retina is also intriguing as an electro-optical device, converting photons into voltages to perform on-the-fly filtering before the signals are sent to our brain. Here, we consider how the advent of stem cell derived in vitro analogs of the retina, termed retina organoids, opens up an exploration of the interplay between optics, electrics, and mechanics in a complex neuronal network, all in a Petri dish. This review presents state-of-the-art retina organoid protocols by emphasizing links to the biochemical and mechanical signals of in vivo retinogenesis. Electrophysiological recording of active signal processing becomes possible as retina organoids generate light sensitive and synaptically connected photoreceptors. Experimental biophysical

tools provide data to steer the development of mathematical models operating at different levels of coarse-graining. In concert, they provide a means to study how mechanical factors guide retina self-assembly. In turn, this understanding informs the engineering of mechanical signals required to tailor the growth of neuronal network morphology. Tackling the complex developmental and computational processes in the retina requires an interdisciplinary endeavor combining experiment and theory, physics, and biology. The reward is enticing: in the next few years, retina organoids could offer a glimpse inside the machinery of simultaneous cellular self-assembly and signal processing, all in an in vitro setting.).

■ **K. Salbaum, E. Shelton, F. Serwane:** *Retina organoids: Window into the biophysics of neuronal systems*; *Biophysics Rev.* 3, 011302; <https://doi.org/10.1063/5.0077014> (2022).

A MULTI-LAYER DEVICE FOR LIGHT-TRIGGERED HYDROGEN PRODUCTION FROM ALKALINE METHANOL

Yiou Wang, En-Ping Yao, Linzhong Wu, **Jochen Feldmann**, and **Jacek Stolarczyk**

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Hydrogen is a clean and sustainable fuel, but its transport and storage, usually in tanks, remain challenging. In contrast, *in situ* production of the required hydrogen from low-cost liquid alcohols ensures the safe storage and transportation of hydrogen before use in, for example, fuel cells. However, a common method involving thermocatalytic alcohol reforming to hydrogen usually requires high-temperature and high-pressure conditions and leads to CO₂ emission ($\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2\uparrow + 3\text{H}_2\uparrow$, $\Delta G = +9$ kJ/mol). Nature not only fixes CO₂ into hydrocarbons via photosynthesis, but also captures it in the form of dissolved CO₃²⁻ ions under moderate conditions, which can be used by shellfish to build up their shelter and finally end up in rocks around the globe.

Inspired by nature, we have developed a thermodynamically favorable reaction ($\text{CH}_3\text{OH} + 2\text{NaOH} \rightarrow \text{Na}_2\text{CO}_3\downarrow + 3\text{H}_2\uparrow$, $\Delta G = -123$ kJ/mol). Under light irradiation and moderate conditions, clean hydrogen is produced from alkaline methanol on *in-situ* loaded Pt/carbon nitride or TiO₂ nanoparticle photocatalysts, releasing neither CO₂ nor CO and capturing carbon in the form of carbonate. We also introduced

a novel multi-layer device to make maximum use of the incident light and the catalyst nanoparticles as active sites. The proposed layered system shows superior performance compared to the commonly used slurry systems without the need for agitation, reaching state-of-the-art hydrogen evolution activities (maximum rate at ca. 1 μmol/s, turnover frequency (TOF) up to 1 800 000 H₂/Pt-h, total turnover number (TTN) of 470 000 over 38 hours), even better than the benchmark systems driven by heat. Such a carbon-neutral and light-triggered process produces hydrogen safely and efficiently, which could enable scalable fabrication and hold promise for broad and practical applications. Moreover, this study offers a pathway to transform a carbon-containing fuel into a carbon-free fuel without releasing CO₂ but capturing carbon as carbonate.

■ **Yiou Wang***, **En-Ping Yao**, **Linzhong Wu**, **Jochen Feldmann***, and **Jacek Stolarczyk***: *A Multi-layer Device for Light-triggered Hydrogen Production from Alkaline Methanol*; *Angewandte Chemie International Edition* 60, 26694, <https://doi.org/10.1002/anie.202109979> (2021).

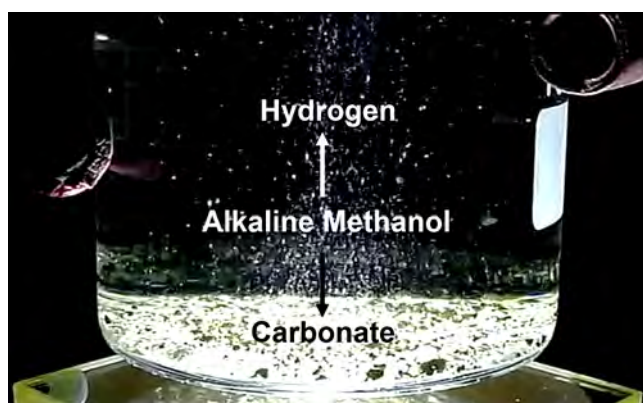


Figure 1. A Pt/CN nanoparticle photocatalyst reforms alkaline methanol to clean hydrogen without CO_x emission.

FOLLOWING THE FATE OF EXCITED STATE PROCESSES IN MULTICHROMOPHORIC SYSTEMS

Tim Schröder, Gordon J. Hedley, Florian Steiner, Sebastian Bange, Theresa Eder, Felix Hofmann, Jakob Schedlbauer, Dirk Laux, Sigurd Höger, **John M. Lupton**, **Philip Tinnefeld**, and Jan Vogelsang

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

The number of emitting units (chromophores) as well as their interactions through exciton diffusion and annihilation processes are key parameters to describe the photophysical characteristics of multichromophoric systems. Similarly, brightness and exciton harvesting efficiency are also important for the performance of materials in optoelectronic

devices. As the chromophores cannot be resolved in space one turns to measure the photon statistics of such materials. A chromophore can emit at maximum one single photon per excitation cycle. The resulting degree of photon antibunching (pAB) is a metric to count the chromophores but exciton-exciton annihilation processes increase the apparent degree of pAB. On short timescales, the singlet-singlet annihilation (SSA) reduces the degree of pAB. On long timescales, collective blinking, due to singlet-triplet annihilation (STA), results in photon bunching but the effect on the degree of pAB was not discussed in literature so far. Here, we tackled both problems in cooperation with the group of John Lupton and Jan Vogelsang from Regensburg University.

We first developed picosecond time resolved anti-bunching (psTRAB) which utilizes the time dependency of SSA.¹ By grouping the photons with respect to their arrival time after pulsed laser excitation, we were able to determine the time dependent probability of consecutive emission of two photons. This allowed extracting both the exact number of chromophores and the time evolution of exciton diffusion and annihilation. We demonstrated psTRAB on well-defined DNA origami structures and applied it to mesoscopic H- and J-type conjugated-polymer aggregates.

Further, we demonstrated how pAB is affected by independent and collective chromophore blinking, which enables us to formulate universal guidelines for pAB interpretation.² We demonstrated our findings on well-defined DNA origami structures and provided two approaches to experimentally distinguish the two blinking mechanisms.

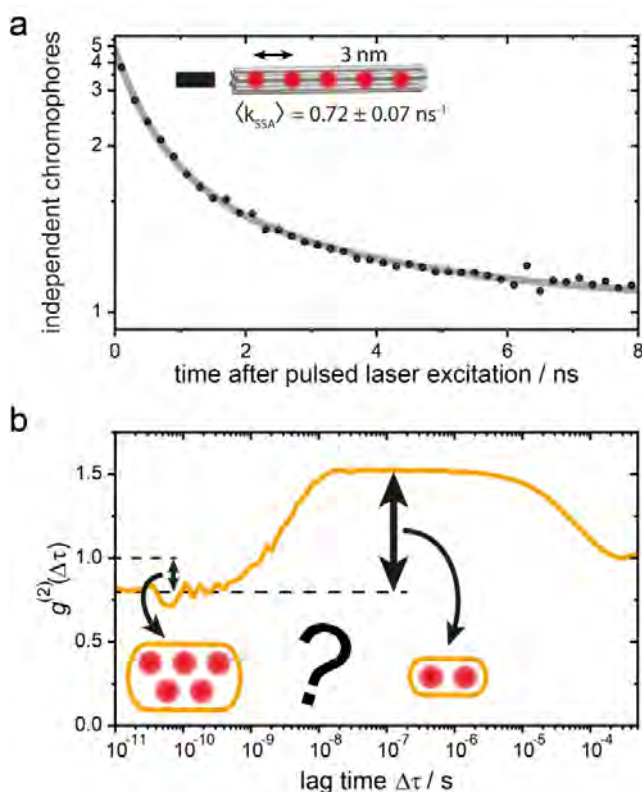


Figure 1. (a) Time evolution of the number of independent emitters as function of the time after pulsed laser excitation on a DNA origami model structure with five organic dyes. psTRAB provides the number of emitters as well as the average SSA kinetics. (b) Simulation of a blinking multichromophoric system. $g^{(2)}(0)$ suggests a five-chromophore system, whereas the normalization to the bunching amplitude suggests a two chromophore system.

■ [1] G. J. Hedley*, T. Schröder*, F. Steiner, T. Eder, F. J. Hofmann, S. Bange, D. Laux, S. Höger, P. Tinnefeld, J. M. Lupton, J. Vogelsang: *Picosecond Time-Resolved Photon Antibunching Measures Nanoscale Exciton Motion and the True Number of Chromophores*; Nat. Commun. 12, 1327, doi.org/10.1038/s41467-021-21474-z (2021).

[2] T. Schröder, S. Bange, J. Schedlbauer, F. Steiner, J. M. Lupton, P. Tinnefeld, J. Vogelsang: *How Blinking Affects Photon Correlations in Multichromophoric Nanoparticles*; ACS Nano 15, 18037–18047, doi.org/10.1021/acsnano.1c06649 (2021).

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A SIMPLE AND GENERAL APPROACH TO GENERATE PHOTOACTIVATABLE DNA PROCESSING ENZYMES

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DNA processing enzymes, such as DNA polymerases and endonucleases, have found many applications in biotechnology, molecular diagnostics, and synthetic biology, among others. The development of enzymes with controllable activity, such as hot-start or light-activatable versions, has boosted their applications and improved the sensitivity and specificity of the existing ones. Most common hot-start strategies employ specific aptamers or antibodies to selectively block the DNA polymerases. The development of such aptamers and antibodies require time-consuming screening of libraries and laborious optimization steps and, after all, they are specific for a certain polymerase. Besides, the unavoidable heating step makes this type of strategy non-viable for mesophilic DNA polymerases. The production of photoactivatable enzymes is commonly based on the incorporation of photosensitive unnatural amino acids and requires detailed structural and mechanistic information of the enzyme. A meticulous study of the case is necessary to place the photosensitive residue in a position that blocks the activity in the off state and releases it only after photoactivation. The latter requires robust knowledge of the enzyme and devising a suitable strategy can be very challenging. Overall, these problems call for strategies of broader application and easier implementation to control the enzymatic activity of DNA processing enzymes. In this project, we devised a simple and general method

to design light-start DNA processing enzymes based on the unspecific competition between an oligonucleotide covalently attached to the enzymes and their substrate (Figure 1). In order to prove its versatility, we applied our method to three DNA polymerases commonly used in biotechnology, including the Phi29 (mesophilic), Taq, and Pfu polymerases, and one restriction enzyme. Light-start enzymes showed suppressed polymerase, exonuclease, and endonuclease activity until they were re-activated by an UV pulse. Furthermore, we applied our enzymes to common molecular biology assays, including a light-started PCR assay, and showed comparable performance to commercial hot-start enzymes.

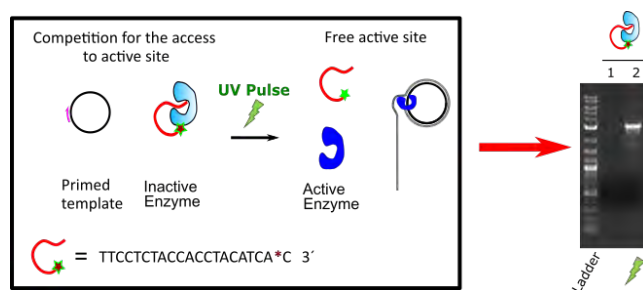


Fig. 1: Schematics of light-start DNA processing enzymes. The attachment of the ssDNA to the enzyme hampers the accessibility of the substrate to the active site leading to enzymatic blockage. Only after photocleavage of the bound DNA the activity is restored. The asterisk (*) denotes a photocleavable linker.

GRAPHENE ENERGY TRANSFER (GET) FOR SINGLE-MOLECULE STUDIES

Izabela Kaminska, Johann Bohlen, Renukka Yaadav, Karolina Zielonka, Patrick Schüler, Mario Raab, Tim Schröder, Jonas Zähringer, Florian Selbach, Florian Steiner, **Evelyn Ploetz**, Stefan Krause, and **Philip Tinnefeld**

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

Graphene, a 2D hexagonal carbon lattice, is known for its superior mechanical and optoelectronic properties. As a result of its zero energy band gap, and frequency independent absorption across the visible spectral range, graphene behaves as a broadband, unbleachable and label-free acceptor. It has been demonstrated, theoretically and experimentally, that the excitation energy is non-radiatively transferred to graphene with a d^{-4} scaling law. Therefore, the measured fluorescence lifetime and intensity of

single emitters may be directly translated into the distance from graphene. Combining these characteristics of graphene with the modularity of self-assembled DNA origami nanopositioners resulted in developing a new type of nanoruler operating at distances up to 40 nm.

Measurements performed with a precision at the single-molecule level required high-quality graphene substrates. We examined 10 methods for graphene transfer and cleaning, while the quality of the sam-

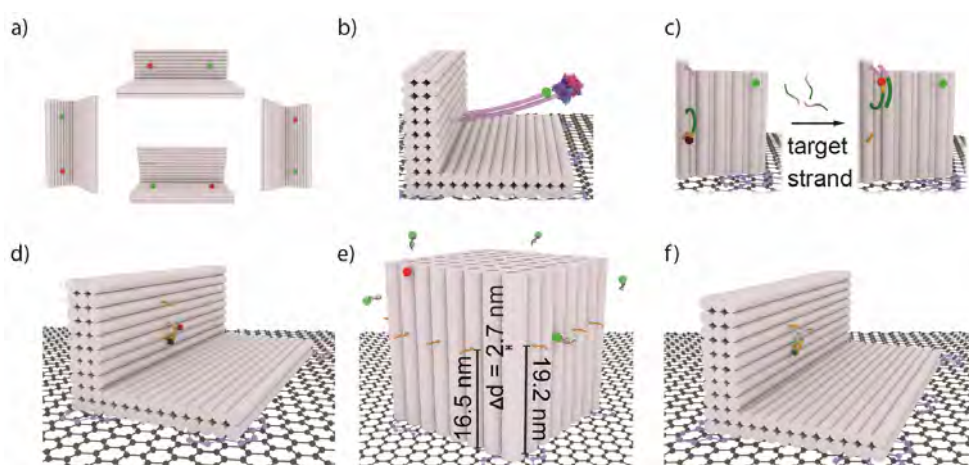


Figure 1. DNA origami structures for GET applications. (a) Multiple possible binding geometries of the L-shaped DNA origami structure to graphene due to additional stacking of the helices. (b) Dynamic investigations and a bioassay were realized by adding a tether to the L-shaped DNA origami structure. (c) As a biosensing assay a dye is more quenched by graphene and after binding of the target strand a higher binding site is accessible (right part of (c)). (d) For FRET measurements, a dynamic DNA origami structure which can transiently bind to two binding sites at different heights. (e) The cubic DNA origami structure contains different binding sites only 2.7 nm apart for super-resolution imaging of the z-distance with DNA-PAINT. (f) Tracking of a dye was realized by equipping the L-shaped DNA origami structure with three different binding sites.

ples was validated by atomic force microscopy, fluorescence lifetime imaging, and Raman spectroscopy. As a result, we established a protocol for the transfer of graphene on glass coverslips with a pristine quality.¹

Further, we equipped graphene-DNA origami hybrids with a whole series of self-designed static and dynamic structures.² In various assays, we determined the orientation of DNA origami structures (Fig. 1a), we sensed target molecules such as streptavidin and DNA (b,c), visualized dynamics of a DNA pointer by combined FRET and graphene energy transfer and achieved superresolution DNA paint with isotropic resolution better than 6 nm (e,f). The range of examples shows the potential of graphene-on-glass coverslips as a versatile platform for single-

molecule biophysics, biosensing, and super-resolution microscopy.

■ [1] S. Krause, E. Plötz, J. Bohlen, P. Schüler, R. Yaadav, F. Selbach, F. Steiner, I. Kaminska, P. Tinnefeld: *Graphene-on-Glass Preparation and Cleaning Methods Characterized by Single-Molecule DNA Origami Fluorescent Probes and Raman Spectroscopy*, ASC NANO, doi.org/10.1021/acsnano.0c08383 (2021).

[2] I. Kaminska, J. Bohlen, R. Yaadav, P. Schüler, M. Raab, T. Schröder, J. Zähringer, K. Zielonka, S. Krause, P. Tinnefeld: *Graphene Energy Transfer for Single-Molecule Biophysics, Biosensing & Superresolution Microscopy*; *Advanced Materials*, doi.org/10.1002/adma.202101099 (2021).

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SINGLE-MOLECULE DIAGNOSTICS WITH DNA ORIGAMI NANOANTENNAS

Viktorija Glembockyte, Kateryna Trofymchuk, Lennart Grabenhorst, Martina Pfeiffer, Cindy Close, Florian Steiner, Renukka Yaadav, Carolin Vietz, Lars Richter, Max L. Schütte, Florian Selbach, Jonas Zähringer, Qingshan Wei, Aydogan Ozcan, Birka Lalkens, Guillermo P. Acuna, Simona Ranallo, Francesco Ricci, Fiona Cole, and **Philip Tinnefeld**

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The possibility to increase fluorescence signals by plasmonic effects opens appealing prospects in the field of single-molecule diagnostics. The last few decades have witnessed a tremendous progress in detecting single molecules, however, to this date, this process requires costly and advanced optical set-ups. To tackle this problem, we utilized the unique advantages of DNA nanotechnology and developed addressable NanoAntennas with Cleared HOtSpots (NACHOS) – DNA origami nanoantennas capable of enhancing the fluorescence signals of single emitters up to few hundred fold.^{1,2} Using NACHOS we could demonstrate detection of single fluorescent molecules with a customary smartphone camera.¹ More importantly, the cleared plasmonic hotspot of NACHOS could be specifically tailored for the incorporation of bioassays. We carried out a single-molecule detection assay for DNA specific to

antibiotic resistant *Klebsiella pneumonia* directly on the portable and battery-powered smartphone microscope illustrating the potential of NACHOS for many exciting applications in point-of-care diagnostic settings. Further work in our group has been also aimed at expanding the scope of NACHOS to diagnostic targets that extend beyond the nucleic acid realm. In collaboration with the group of Francesco Ricci at the University of Rome, we also combined NACHOS with label-free antibody detection by incorporating a nanoswitch in the plasmonic hotspot of the nanoantenna.³ The nanoswitch contains two antigens that are displaced by antibody binding, thereby eliciting a fluorescent signal. The integration of an anti-digoxygenin antibody nanoswitch in the hotspot of the DNA nanoantennas results in further amplification of fluorescence signal enabling detection of

single antibodies on the portable smartphone microscope.

■ [1] K. Trofymchuk, V. Glembockyte, L. Grabenhorst, F. Steiner, C. Vietz, C. Close, M. Pfeiffer, L. Richter, M. L. Schütte, F. Selbach, R. Yaadav, J. Zähringer, Q. Wei, A. Ozcan, B. Lalkens, G. P. Acuna, P. Tinnefeld: *Addressable nanoantennas with cleared hotspots for single-molecule detection on a portable smartphone microscope*; Nature Communications, doi10.1038/s41467-021-21238-9 (2021).

[2] V. Glembockyte, L. Grabenhorst, K. Trofymchuk, P. Tinnefeld: *DNA Origami Nanoantennas for Fluorescence Enhancement*; Accounts of Chemical Research, doi10.1021/acs.accounts.1c00307 (2021).

[3] M. Pfeiffer, K. Trofymchuk, S. Ranallo, F. Ricci, F. Steiner, F. Cole, V. Glembockyte, P. Tinnefeld: *Single antibody detection in a DNA origami nanoantenna*; iScience, doi10.1016/j.isci.2021.103072 (2021).

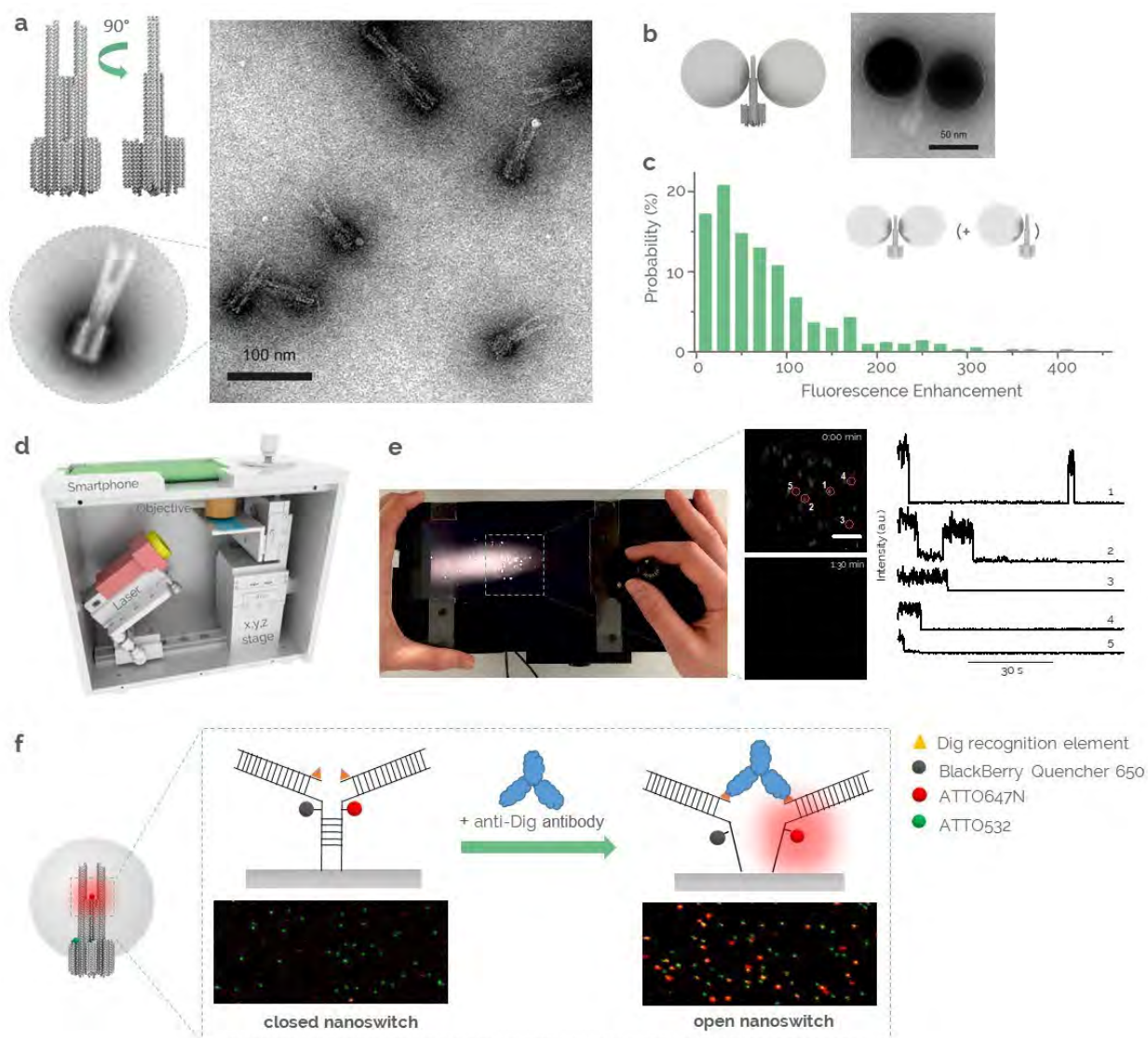


Figure 1. (a) DNA origami structure used to scaffold addressable NanoAntennas with Cleared HOtSpots (NACHOS); (b) Structure of a full DNA origami nanoantenna containing two 60-nm gold nanoparticles; (c) Fluorescence enhancement values obtained for NACHOS containing two 100-nm silver nanoparticles; (d) Sketch of the portable smartphone-based microscope used to detect single fluorescent molecules with the help of NACHOS; (e) Picture of the portable microscope (left) and images as well as single-molecule trajectories acquired on the smartphone camera (right); (f) Label-free assay to detect single-antibodies with DNA nanoantennas by incorporation of the nanoswitch in the plasmonic hotspot.

MEMBRANE POTENTIAL SENSORS WITH SINGLE-MOLECULE SENSITIVITY ENABLED BY DNA NANOTECHNOLOGY

Sarah E. Ochmann, Himanshu Joshi, Ece Büber, Henri G. Franquelim, Tim Schröder, Clara M. Schulz, Pierre Stegemann, Barbara Saccà, Ulrich F. Keyser, Aleksei Aksimentiev, and **Philip Tinnefeld**

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As the barrier between the interior and exterior environments of a cell, the cell membrane is involved in various biological processes and measuring electrical membrane potentials is a key feature of neuronal research. Still, improved optical membrane potential sensors that are not genetically encoded are highly desired.

We used the DNA origami technique to modularly overcome different challenges of voltage sensors such as membrane targeting and placing a sensory element, and established a new family of FRET (fluorescence resonance energy transfer) based non-genetically encoded voltage-sensing strategies that allows sensing on the single-molecule level. The

FRET sensor element employs a new principle using a hydrophobic ATTO647N dye that anchors the sensor unit in the membrane (see Figure 1a). A donor dye is placed on negatively charged DNA linkers that are attached to the DNA origami. Depending on the potential, the flexible element with the donor changes its position relative to the FRET acceptor in the membrane yielding a FRET change that is read out on single FRET pairs with a change of $\sim 5\%$ for $\Delta\Psi = 100$ mV. Besides transmembrane potentials,¹ a similar principle was also employed to study surface potentials induced by the composition of lipids with different charges in large unilamellar vesicles (Figure 1b).²

Here, we achieved a change in energy transfer of $\sim 10\%$ points between uncharged and highly charged membranes and demonstrated a quantitative relation between the surface charge and the energy transfer. We hope to apply these sensors in biological systems in the future.

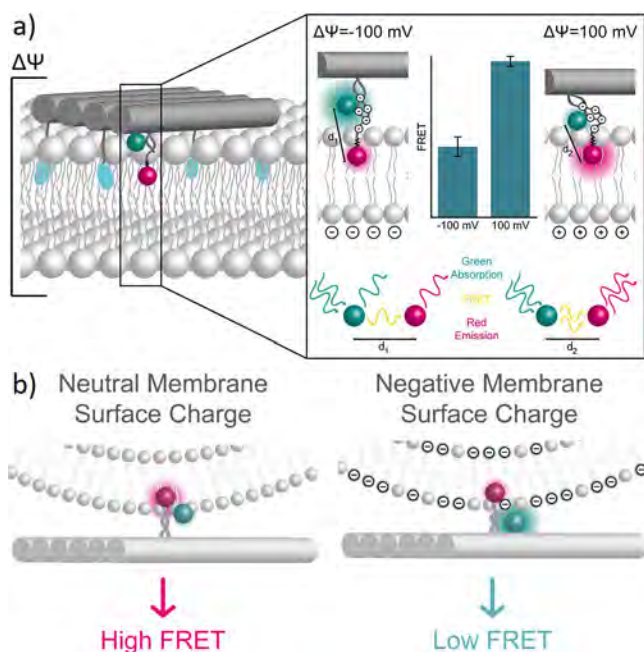


Figure 1. (a) Sketch of DNA origami sensor for transmembrane potentials. Depending on the potential the negatively charged sensor above the membrane changes its position which is read out by FRET. (b) Sketch of a similar DNA origami sensor for sensing membrane charges.

■ [1] S. E. Ochmann, H. Joshi, E. Büber, H. G. Franquelim, P. Stegemann, B. Saccà, U. F. Keyser, A. Aksimentiev, P. Tinnefeld: *DNA Origami Voltage Sensors for Transmembrane Potentials with Single-Molecule Sensitivity*; *Nano Lett.* 21(20):8634-8641. doi: 10.1021/acs.nanolett.1c02584 (2021).

[2] S. E. Ochmann, T. Schröder, C. M. Schulz, P. Tinnefeld: *Quantitative Single-Molecule Measurements of Membrane Charges with DNA Origami Sensors*; *Analytical Chemistry*, doi10.1021/acs.analchem.1c05092 (2021).

TIP-COUPLING AND ARRAY EFFECTS OF GOLD NANOANTENNAS IN NEAR-FIELD MICROSCOPY

Rebecca Büchner, Thomas Weber, Lucca Kühner, **Stefan A. Maier**, and **Andreas Tittl**

■ <https://www.hybridplasmonics.org>

Scattering-type scanning near-field optical microscopy (s-SNOM) is one of the predominant techniques for nanoscale characterization of optical properties. The optical response of nanoantennas in s-SNOM is highly sensitive to their environment, including influences of the probing tip or neighboring resonators. To minimize tip-related perturbations, dielectric tips are commonly employed, although they provide a comparatively weak scattering signal.

In this research, we show that when using metallic tips, it is possible to select between distinct weak and strong tip-antenna coupling regimes by careful tailoring of the illumination condition and resonator orientation. This enables the use of highly scattering metallic instead of dielectric tips for mapping plasmonic modes with commensurate much higher signal strengths. This is a particular advantage for the retrieval of near-field spectra, which simultaneously require high near-field signals and unperturbed field patterns. We leverage our approach to analyze collective effects of nanoantenna arrays, phenomena that are well understood in the optical far field, but have not been studied extensively in the near field. Probing the dependence of the optical response on array field size, we identify three regimes: single rod regime, intermediate regime, and array-like regime. We show that these array effects give rise to characteristic spectral features that arise from a complex interplay of radiative coupling and plasmon hybridization.

These results provide evidence that long-range interactions of antennas also influence the local optical response that is probed in s-SNOM and demonstrate how collective resonances emerge from single building blocks, providing guidelines for optimized array designs for near- and far-field applications. In addition,

this paper has appeared on the Front Cover of ACS Photonics, bringing the work to the attention of a wider audience.

■ **R. Büchner, T. Weber, L. Kühner, S. A. Maier, and A. Tittl:** *Tip Coupling and Array Effects of Gold Nanoantennas in Near-Field Microscopy*; ACS Photonics 8, 3486–3494 (2021).

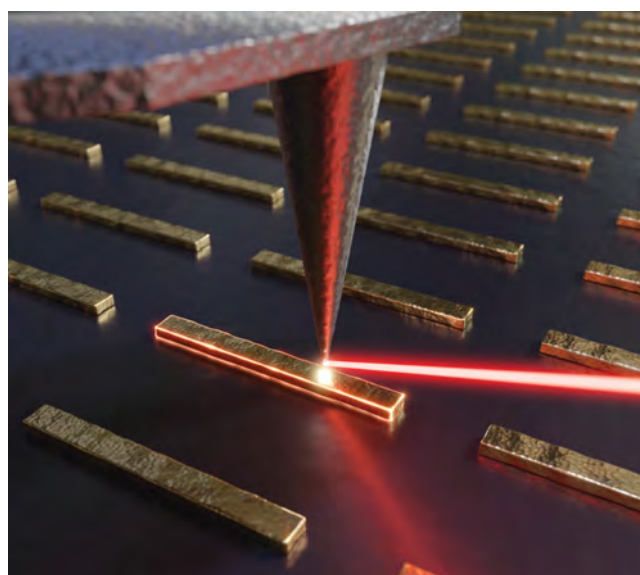


Figure 1. In the near-field microscopy of resonant nanoantenna systems, distinct weak and strong tip-antenna coupling regimes can be obtained by careful tailoring of the illumination condition and resonator orientation. This approach enables greater flexibility in the choice of tip material as well as improved signal-to-noise ratios for investigations of nanophotonic systems.

DARK AND BRIGHT EXCITONS IN HALIDE PEROVSKITE NANOPATELETS

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Semiconductor nanoplatelets (NPLs), with their large exciton binding energy, narrow photoluminescence (PL), and absence of dielectric screening for photons emitted normal to the NPL surface, could be expected to become the fastest luminophores amongst all colloidal nanostructures. However, super-fast emission is suppressed by a dark (optically passive) exciton ground state, substantially split from a higher-lying bright (optically active) state. Here, the exciton fine structure in 2–8 monolayer (ML) thick $\text{Cs}_{n-1}\text{Pb}_n\text{Br}_{3n+1}$ NPLs is revealed by merging temperature-resolved PL spectra and time-resolved PL decay with an effective mass model taking quantum confinement and dielectric confinement anisotropy into account. This approach exposes a thickness-dependent bright–dark exciton splitting reaching 32.3 meV for the 2 ML NPLs. The model also reveals a 5–16 meV splitting of the bright exciton states with transition dipoles polarized parallel and perpendicular to the NPL surfaces, the order of which is reversed for the thinnest NPLs, as confirmed by TR-PL measurements. Accordingly, the individual bright states must be taken into account, while the dark exciton state strongly affects the optical properties of the thinnest NPLs even at room temperature. Significantly, the derived model can be generalized for any isotropically or anisotropically confined nanostructure.

■ **M. Gramlich, M. W. Swift, C. Lampe, J. L. Lyons, M. Döblinger, A. L. Efros, P. C. Sercel, A. S. Urban:** *Dark and Bright Excitons in Halide Perovskite Nanoplatelets*; *Advanced Science*, <https://doi.org/10.1002/advs.202103013> (2021).

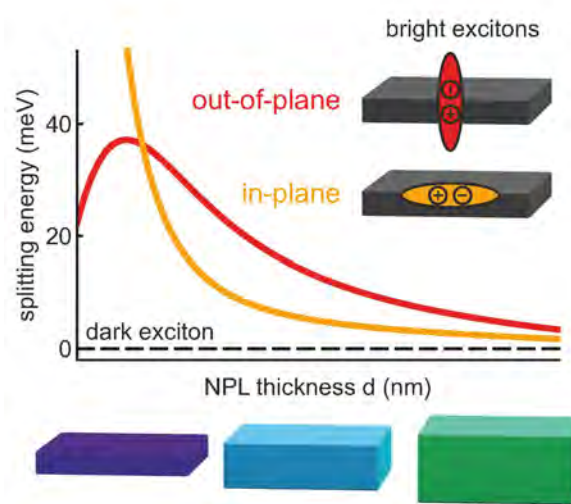


Figure 1. 2D semiconductor nanoplatelets can enable faster and more efficient light-emitting devices. For this, a detailed understanding of their energetic structure is paramount. Here, the thickness-dependent exciton fine structure of nanoplatelets is deduced by merging temperature and time-resolved photoluminescence spectroscopy with a novel effective mass model, considering anisotropic quantum and dielectric confinement. Relevantly, the model can be generalized for any nanostructure.

THE ACTIVITY OF THE INTRINSICALLY WATER-SOLUBLE ENZYME ADAMTS13 CORRELATES WITH THE MEMBRANE STATE WHEN BOUND TO A PHOSPHOLIPID BILAYER

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- The temperature dependence of the activity of ADAMTS13 when bound to a lipid bilayer shows a distinct maximum close to the main phase transition temperature T_m of the membrane.
- Changing the carbon chain length of the used lipid, and thus T_m , shifts the activity maximum to the new T_m .
- Comparing the activity at a constant temperature for three different membranes in the gel phase, the fluid phase and at the transition underline the role of the membrane state for the enzyme activity.
- These results are perfectly in line with the concept that increased fluctuations close to a phase transition are crucial for catalysis.

■ A. Kamenac, T. Obser, A. Wixforth, M. F. Schneider, and C. Westerhausen: *The activity of the intrinsically water-soluble enzyme ADAMTS13 correlates with the membrane state when bound to a phospholipid bilayer*; Scientific Reports 11, 24476, <https://doi.org/10.1038/s41598-021-04083-0> (2021).

Matthias F. Schneider: *Living systems approached from physical principles*; Progress in Biophysics and Molecular Biology 162: 2-25. <https://doi.org/10.1016/j.pbiomolbio.2020.10.001>

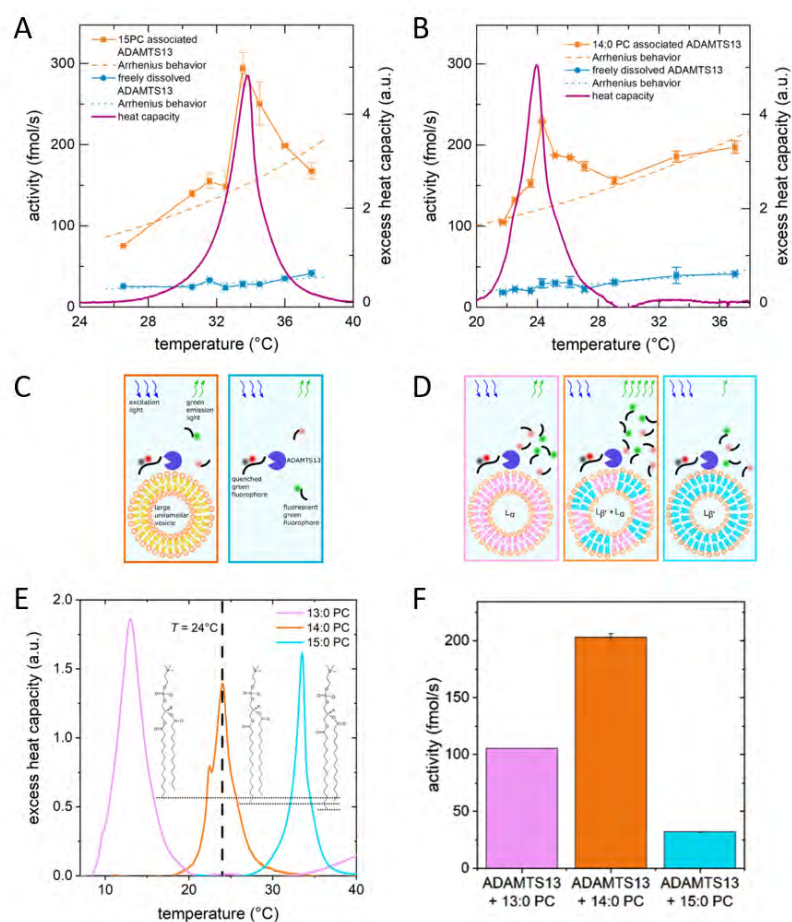


Figure 1. Activity of the water soluble enzyme ADAMTS13 bound to lipid membranes (orange) and freely dissolved (blue) for PC liposomes of different chain length. A) 15:0 PC and B) 14:0 PC. C) Illustration of the experimental design. One well (left, orange frame) contains the substrate, enzyme, and vesicles, whereas in the other (right, blue frame), the vesicles are substituted by buffer. The assay is based on fluorescence-resonance-energy-transfer (FRET). Embedded ALEXA fluorochromes in the A2 domain of VWF (Von-Willebrand-Factor) are decoupled after cleaving of the substrate, this leads to an increase of the green fluorescence. D) ADAMTS13 (purple circle segment) was attached to three different liposomes: 13:0 PC (left), 15:0 PC (right), and 14:0 PC (middle), FRET-substrate was added (black with colored dots). At 24 °C, the phase states of the liposomes are L_{α} , L_{β} , and in coexistence, respectively, as illustrated by their acyl-chain shape and color. E) Excess heat capacity of liposomes of three phosphocholines with different acyl-chain lengths. At 24 °C all three membranes are in a different phase state: 13:0 PC is L_{α} , 15:0 PC is L_{β} , and 14:0 PC is in the coexistence regime. F) ADAMTS13 activity determined from experiments as illustrated in D) at 24°C.

LINKER EXCHANGE VIA MIGRATION ALONG THE BACKBONE IN METAL-ORGANIC FRAMEWORKS

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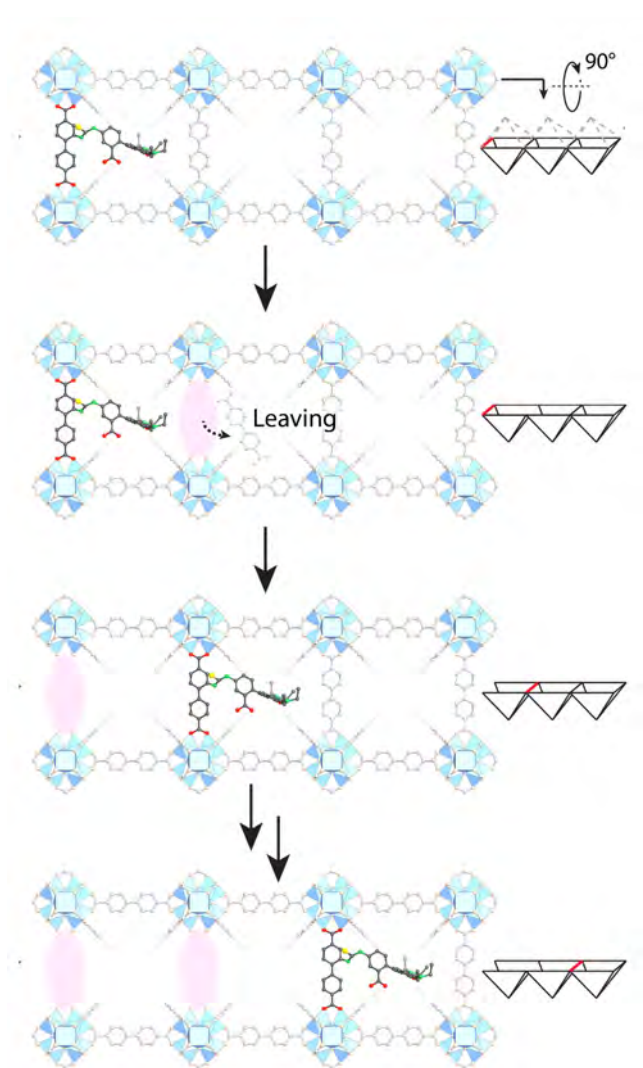
In a long standing collaboration with the group of Stefan Wuttke, we investigated the process of linker exchange in Metal-Organic-Frameworks (MOFs). MOFs are a relatively new class of highly porous material that can be easily manipulated for designing a number of functionalities. It was recently noticed that the linkers used to form MOFs can also be exchanged after synthesis, enabling new functionalities that were not previously possible. In this tour-de-force investigation over several years, we discovered that it was possible to exchange linkers that are larger than the pore size of the MOFs via a new mechanism. The key findings of our work are:

1) Post synthetic exchange of linkers larger than the windows in the MOFs is possible via a new mechanism termed "Through Backbone Diffusion" where the new linkers diffuse through the MOFs framework by replacing adjacent linkers.

2) Through Backbone Diffusion proceeds from the outside of the crystal towards the center and leads to an accumulation of defects in the MOFs in the wake of this diffusion.

3) We demonstrate that it is possible to incorporate large, sophisticated guest molecules such as catalysts or biomolecules within a formed MOF framework, opening the possibility for manufacturing MOFs with new functionalities.

■ **N. Al Danaf, W. Schrimpf, P. Hirschle, D. C. Lamb, Z. Ji, and S. Wuttke:** *Linker Exchange via Migration along the Backbone in Metal-Organic Frameworks*; *J Am Chem Soc* 143, 10541 (2021).





**SELECTED
PUBLICATIONS**

- Al Danaf, N., W. Schrimpf, P. Hirschle, D. C. Lamb, Z. Ji and S. Wuttke:** Linker Exchange via Migration along the Backbone in Metal-Organic Frameworks. *Journal of the American Chemical Society* 143(28): 10541-10546 (2021).
- Bangerter, F. H., M. Glasbrenner and C. Ochsenfeld:** Low-Scaling Tensor Hypercontraction in the Cholesky Molecular Orbital Basis Applied to Second-Order Moller-Plesset Perturbation Theory. *Journal of Chemical Theory and Computation* 17(1): 211-221 (2021).
- Beetz, M., S. Haringer, P. Elsasser, J. Kampmann, L. Sauerland, F. Wolf, M. Gunther, A. Fischer and T. Bein:** Ultra-Thin Protective Coatings for Sustained Photoelectrochemical Water Oxidation with Mo:BiVO₄. *Advanced Functional Materials* 31(45) (2021).
- Benli-Hoppe, T., S. G. Ozturk, O. Ozturk, S. Berger, E. Wagner and M. Yazdi:** Transferrin Receptor Targeted Polyplexes Completely Comprised of Sequence-Defined Components. *Macromolecular Rapid Communications* 43, 2100602 (2022).
- Berger, R. M. L., J. M. Weck, S. M. Kempe, O. Hill, T. Liedl, J. O. Radler, C. Monzel and A. Heuer-Jungemann:** Nanoscale FasL Organization on DNA Origami to Decipher Apoptosis Signal Activation in Cells. *Small* 17(26) (2021).
- Bessinger, D., K. Muggli, M. Beetz, F. Auras and T. Bein:** Fast-Switching Vis-IR Electrochromic Covalent Organic Frameworks. *Journal of the American Chemical Society* 143(19): 7351-7357 (2021).
- Bohm, D., M. Beetz, C. Gebauer, M. Bernt, J. Schroter, M. Kornherr, F. Zoller, T. Bein and D. Fattakhova-Rohlfing:** Highly conductive titania supported iridium oxide nanoparticles with low overall iridium density as OER catalyst for large-scale PEM electrolysis. *Applied Materials Today* 24 (2021).
- Bravo, J. P. K., K. Bartnik, L. Venditti, J. Acker, E. H. Gail, A. Colyer, C. Davidovich, D. C. Lamb, R. Tuma, A. N. Calabrese and A. Borodavka:** Structural basis of rotavirus RNA chaperone displacement and RNA annealing. *Proceedings of the National Academy of Sciences of the United States of America* 118(41) (2021).
- Buchner, R., T. Weber, L. Kuhner, S. A. Maier and A. Tittl:** Tip Coupling and Array Effects of Gold Nanoantennas in Near-Field Microscopy. *Acs Photonics* 8(12): 3486-3494 (2021).
- Buyruk, A., D. Blatte, M. Gunther, M. A. Scheel, N. F. Hartmann, M. Doblinger, A. Weis, A. Hartschuh, P. Müller-Buschbaum, T. Bein and T. Ameri:** 1,10-Phenanthroline as an Efficient Bifunctional Passivating Agent for MAPbI(3) Perovskite Solar Cells. *ACS Applied Materials & Interfaces* 13(28): 32894-32905 (2021).
- Cao, J. F., O. T. Zaremba, Q. Lei, E. Ploetz, S. Wuttke and W. Zhu:** Artificial Bioaugmentation of Biomacromolecules and Living Organisms for Biomedical Applications. *ACS Nano* 15(3): 3900-3926 (2021).
- Chen, K. J., M. Q. Cao, Y. Y. Lin, J. W. Fu, H. X. Liao, Y. J. Zhou, H. M. Li, X. Q. Qiu, J. H. Hu, X. S. Zheng, M. Shakouri, Q. F. Xiao, Y. F. Hu, J. Li, J. L. Liu, E. Cortes and M. Liu:** Ligand Engineering in Nickel Phthalocyanine to Boost the Electrocatalytic Reduction of CO₂. *Advanced Functional Materials* (2021).
- Claude, K. L., D. Bureik, P. Adarska, A. Singh, K. M. Schmoller and D. Chatzitheodoridou:** Transcription coordinates histone amounts and genome content. *Nature Communications* 12(1) (2021).
- Ejsmont, A., J. Andreo, A. Lanza, A. Galarda, L. Macreadie, S. Wuttke, S. Canossa, E. Ploetz and J. Goscianska:** Applications of reticular diversity in metal-organic frameworks: An ever-evolving state of the art. *Coordination Chemistry Reviews* 430 (2021).

* CeNS Publication Award 2021

- Ertelt, M. J., H. Hilbig, C. U. Grosse and O. Lieleg:** Small Pores, Big Impact-Controlling the Porosity Allows for Developing More Sustainable Construction Materials. *ACS Sustainable Chemistry & Engineering* 9(39): 13188-13195 (2021).
- Feldmann, S., T. Neumann, R. Ciesielski, R. H. Friend, A. Hartschuh and F. Deschler:** Tailored Local Bandgap Modulation as a Strategy to Maximize Luminescence Yields in Mixed-Halide Perovskites. *Advanced Optical Materials* 9(18) (2021).
- Forg, M., A. S. Baimuratov, S. Y. Kruchinin, I. A. Vovk, J. Scherzer, J. Forste, V. Funk, K. Watanabe, T. Taniguchi and A. Högele:** Moire excitons in MoSe_2 - WSe_2 heterobilayers and heterotrayers. *Nature Communications* 12(1) (2021).
- Freitag, M., D. Kamp, M. Synakewicz and J. Stigler:** Identification and correction of misalignment artifacts based on force noise for optical tweezers experiments. *Journal of Chemical Physics* 155(17) (2021).
- Freund, R., O. Zaremba, M. Dinca, G. Arnauts, R. Ameloot, G. Skorupskii, A. Bavykina, J. Gascon, A. Ejsmont, J. Goscianska, M. Kalmutzki, U. Lächelt, E. Ploetz, C. S. Diercks and S. Wuttke:** The Current Status of MOF and COF Applications. *Angewandte Chemie-International Edition* 60(45): 23975-24001 (2021).
- Frey, L., J. J. Jarju, L. M. Salonen and D. D. Medina:** Boronic-acid-derived covalent organic frameworks: from synthesis to applications. *New Journal of Chemistry* 45(33): 14879-14907 (2021).
- Fuchs, A., P. Mannhardt, P. Hirschle, H. Z. Wang, I. Zaytseva, Z. Ji, O. Yaghi, S. Wuttke and E. Ploetz:** Single Crystals Heterogeneity Impacts the Intrinsic and Extrinsic Properties of Metal-Organic Frameworks. *Advanced Materials* 34(3) (2022).
- Funk, V., K. Wagner, E. Wietek, J. D. Ziegler, J. Forste, J. Lindlau, M. Förg, K. Watanabe, T. Taniguchi, A. Chernikov and A. Högele:** Spectral asymmetry of phonon sideband luminescence in monolayer and bilayer WSe_2 . *Physical Review Research* 3(4) (2021).
- Geiger, F., J. Acker, G. Papa, X. Y. Wang, W. E. Arter, K. L. Saar, N. A. Erkamp, R. Z. Qi, J. P. Bravo, S. Strauss, G. Krainer, O. R. Burrone, R. Jungmann, T. P. J. Knowles, H. Engelke and A. Borodavka:** Liquid-liquid phase separation underpins the formation of replication factories in rotaviruses. *Embo Journal* 40(21) (2021).
- Girard, E. B., A. Fuchs, M. Kaliwoda, M. Lasut, E. Ploetz, W. W. Schmahl and G. Worheide:** Sponges as bioindicators for microparticulate pollutants? *Environmental Pollution* 268 (2021).
- Gonzalez, I. R. R., P. I. R. Pincheira, A. M. S. Macedo, L. D. Menezes, A. S. L. Gomes and E. P. Raposo:** Intensity distribution in random lasers: comparison between a stochastic differential model of interacting modes and random phase sum-based models. *Journal of the Optical Society of America B-Optical Physics* 38(8): 2391-2398 (2021).
- Gramlich, M., M. W. Swift, C. Lampe, J. L. Lyons, M. Dobliger, A. L. Efros, P. C. Sercel and A. S. Urban:** Dark and Bright Excitons in Halide Perovskite Nanoplatelets. *Advanced Science* 9(5) (2022).
- Grunenberg, L., G. Savasci, M. W. Terban, V. Duppel, I. Moudrakovski, M. Etter, R. E. Dinnebier, C. Ochsenfeld and B. V. Lotsch:** Amine-Linked Covalent Organic Frameworks as a Platform for Postsynthetic Structure Interconversion and Pore-Wall Modification. *Journal of the American Chemical Society* 143(9): 3430-3438 (2021).
- Gunther, M., D. Blatte, A. L. Oechsle, S. S. Rivas, A. A. Y. Amin, P. Müller-Buschbaum, T. Bein and T. Ameri:** Increasing Photostability of Inverted Nonfullerene Organic Solar Cells by Using Fullerene Derivative Additives. *ACS Applied Materials & Interfaces* 13(16): 19072-19084 (2021).

- Guo, J. M., Y. L. Yu, W. Zhu, R. E. Serda, S. Franco, L. Wang, Q. Lei, J. O. Agola, A. Nouredine, E. Ploetz, S. Wuttke and C. J. Brinker:** Modular Assembly of Red Blood Cell Superstructures from Metal-Organic Framework Nanoparticle-Based Building Blocks. *Advanced Functional Materials* 31(10) (2021).
- Heuer-Jungemann, A. and V. Linko:** Engineering Inorganic Materials with DNA Nanostructures. *ACS Central Science* 7(12): 1969-1979 (2021).
- Hüttenhofer, L., A. Tittl, L. Kuhner, E. Cortes and S. A. Maier:** Anapole-Assisted Absorption Engineering in Arrays of Coupled Amorphous Gallium Phosphide Nanodisks. *ACS Photonics* 8(5): 1469-1476 (2021).
- L. Hüttenhofer, M. Golibrzuch, O. Bienek, F. J. Wendisch, R. Lin, M. Becherer, I. D. Sharp, S. A. Maier and E. Cortés:** Metasurface Photoelectrodes for Enhanced Solar Fuel Generation; *Advanced Energy Materials*, <https://doi.org/10.1002/aenm.202102877> (2021).
- Ianeselli, A., D. Tetiker, J. Stein, A. Kühnlein, C. B. Mast, D. Braun and T. Y. D. Tang:** Non-equilibrium conditions inside rock pores drive fission, maintenance and selection of coacervate protocells. *Nature Chemistry* 14(1): 32 (2022).
- Ijas, H., B. X. Shen, A. Heuer-Jungemann, A. Keller, M. A. Kostianen, T. Liedl, J. A. Ihalainen and V. Linko:** Unraveling the interaction between doxorubicin and DNA origami nanostructures for customizable chemotherapeutic drug release. *Nucleic Acids Research* 49(6): 3048-3062 (2021).
- Illes, B., A. Fuchs, F. Gegenfurtner, E. Ploetz, S. Zahler, A. M. Vollmar and H. Engelke:** Spatio-selective activation of nuclear translocation of YAP with light directs invasion of cancer cell spheroids. *IScience* 24(3) (2021).
- Kaltenecker, K. J., T. Golz, E. Bau and F. Keilmann:** Infrared-spectroscopic, dynamic near-field microscopy of living cells and nanoparticles in water. *Scientific Reports* 11(1) (2021).
- Kamenac, A., F. L. Schilberth, E. Wagner, A. Wixforth, U. Lächelt and C. Westerhausen:** Transient Permeabilization of Living Cells: Combining Shear Flow and Acoustofluidic Trapping for the Facilitated Uptake of Molecules. *Processes* 9(6) (2021).
- Kaminska, I., J. Bohlen, R. Yaadav, P. Schüler, M. Raab, T. Schröder, J. Zähringer, K. Zielonka, S. Krause and P. Tinnefeld:** Graphene Energy Transfer for Single-Molecule Biophysics, Biosensing, and Super-Resolution Microscopy. *Advanced Materials* 33(24) (2021).
- Karg, C. A., S. J. Wang, N. Al Danaf, R. P. Pember-ton, D. Bernard, M. Kretschmer, S. Schneider, T. Zisis, A. M. Vollmar, D. C. Lamb, S. Zahler and S. Moser:** Tetrapyrrolic Pigments from Heme- and Chlorophyll Breakdown are Actin-Targeting Compounds. *Angewandte Chemie-International Edition* 60(41): 22578-22584 (2021).
- Kepic, P., F. Ligmajer, M. Hrton, H. R. Ren, L. D. Menezes, S. A. Maier and T. Sikola:** Optically Tunable Mie Resonance VO₂ Nanoantennas for Metasurfaces in the Visible. *Acs Photonics* 8(4): 1048-1057 (2021).
- Kesici, M. Z., P. Tinnefeld and A. M. Vera:** A simple and general approach to generate photoactivatable DNA processing enzymes. *Nucleic Acids Res* (2021).
- Kolbeck, P. J., W. Vanderlinden, G. Gemmecker, C. Gebhardt, M. Lehmann, A. Lak, T. Nicolaus, T. Cordes and J. Lipfert:** Molecular structure, DNA binding mode, photophysical properties and recommendations for use of SYBR Gold. *Nucleic Acids Research* 49(21): 12601-12602 (2021).
- Konrad, S. F., W. Vanderlinden, W. Frederickx, T. Brouns, B. H. Menze, S. De Feyter and J. Lipfert:** High-throughput AFM analysis reveals unwrapping pathways of H3 and CENP-A nucleosomes. *Nanoscale* 13(10): 5435-5447 (2021).

* CeNS Publication Award 2021

- Koschnick, C., R. Staglich, T. Scholz, M. W. Terban, A. von Mankowski, G. Savasci, F. Binder, A. Schokel, M. Etter, J. Nuss, R. Siegel, L. S. Germann, C. Ochsenfeld, R. E. Dinnebier, J. Senker and B. V. Lotsch:** Understanding disorder and linker deficiency in porphyrinic zirconium-based metal-organic frameworks by resolving the Zr_8O_6 cluster conundrum in PCN-221. *Nature Communications* 12(1) (2021).
- Krause, S., E. Ploetz, J. Bohlen, P. Schüler, R. Yaadav, F. Selbach, F. Steiner, I. Kamin-ska and P. Tinnefeld:** Graphene-on-Glass Preparation and Cleaning Methods Characterized by Single-Molecule DNA Origami Fluorescent Probes and Raman Spectroscopy. *Acs Nano* 15(4): 6430-6438 (2021).
- Kreppel, A. and C. Ochsenfeld:** The Enzymatic Decarboxylation Mechanism of 5-Carboxy Uracil: A Comprehensive Quantum Chemical Study. *Journal of Chemical Theory and Computation* 17(1): 96-104 (2021).
- Kroger, J., A. Jimenez-Solano, G. Savasci, V. W. H. Lau, V. Duppel, I. Moudrakovski, K. Kuster, T. Scholz, A. Gouder, M. L. Schreiber, F. Podjaski, C. Ochsenfeld and B. V. Lotsch:** Morphology Control in 2D Carbon Nitrides: Impact of Particle Size on Optoelectronic Properties and Photocatalysis. *Advanced Functional Materials* 31(28) (2021).
- Kroger, J., A. Jimenez-Solano, G. Savasci, P. Rovo, I. Moudrakovski, K. Kuster, H. Schlomberg, H. A. Vignolo-Gonzalez, V. Duppel, L. Grunenber, C. B. Dayan, M. Sitti, F. Podjaski, C. Ochsenfeld and B. V. Lotsch:** Interfacial Engineering for Improved Photocatalysis in a Charge Storing 2D Carbon Nitride: Melamine Functionalized Poly(heptazine imide). *Advanced Energy Materials* 11(6) (2021).
- Kroger, J., F. Podjaski, G. Savasci, I. Moudrakovski, A. Jimenez-Solano, M. W. Terban, S. Bette, V. Duppel, M. Joos, A. Senocrate, R. Dinnebier, C. Ochsenfeld and B. V. Lotsch:** Conductivity Mechanism in Ionic 2D Carbon Nitrides: From Hydrated Ion Motion to Enhanced Photocatalysis. *Advanced Materials* 34(7) (2022).
- Kudella, P. W., A. V. Tkachenko, A. Salditt, S. Maslov and D. Braun:** Structured sequences emerge from random pool when replicated by templated ligation. *Proceedings of the National Academy of Sciences of the United States of America* 118(8) (2021).
- F. B. Kugler, S.-S. B. Lee and J. von Delft:** Multi-point Correlation Functions: Spectral Representation and Numerical Evaluation; *Physical Review X*, 10.1103/PhysRevX.11.041006 (2021).
- Kuhne, J., J. Wang, T. Weber, L. Kuhner, S. A. Maier and A. Tittl:** Fabrication robustness in BIC metasurfaces. *Nanophotonics* 10(17): 4305-4312 (2021).
- Kühnlein, A., S. A. Lanzmich and D. Braun:** tRNA sequences can assemble into a replicator. *Elife* 10 (2021).
- Lackinger, M.:** Synthesis on inert surfaces. *Dalton Transactions* 50(29): 10020-10027 (2021).
- Lerner, E., A. Barth, J. Hendrix, B. Ambrose, V. Birkedal, S. C. Blanchard, R. Borner, H. S. Chung, T. Cordes, T. D. Craggs, A. A. Deniz, J. J. Diao, J. Y. Fei, R. L. Gonzalez, I. V. Gopich, T. Ha, C. A. Hanke, G. Haran, N. S. Hatzakis, S. Hohng, S. C. Hong, T. Hugel, A. Ingargiola, C. Joo, A. N. Kapanidis, H. D. Kim, T. Laurence, N. K. Lee, T. H. Lee, E. A. Lemke, E. Margeat, J. Michaelis, X. Michalet, S. Myong, D. Nettels, T. O. Peulen, E. Ploetz, Y. Razvag, N. C. Robb, B. Schuler, H. Soleimaninejad, C. Tang, R. Vafabakhsh, D. C. Lamb, C. A. M. Seidel and S. Weiss:** FRET-based dynamic structural biology: Challenges, perspectives and an appeal for open-science practices. *Elife* 10 (2021).
- Levacic, A. K., S. Berger, J. Muller, A. Wegner, U. Lächelt, C. Dohmen, C. Rudolph and E. Wagner:** Dynamic mRNA polyplexes benefit from bioreducible cleavage sites for in vitro and in vivo transfer. *Journal of Controlled Release* 339: 27-40 (2021).

- Lobe, S., A. Bauer, S. Uhlenbruck and D. Fattakhova-Rohlfing:** Physical Vapor Deposition in Solid-State Battery Development: From Materials to Devices. *Advanced Science* 8(11) (2021).
- Loy, D. M., R. Krzysztan, U. Lächelt, J. O. Radler and E. Wagner:** Controlling Nanoparticle Formulation: A Low-Budget Prototype for the Automation of a Microfluidic Platform. *Processes* 9(1) (2021).
- Luo, J., J. Schmaus, M. C. Cui, E. Horterer, U. Wilk, M. Hohn, M. Dather, S. Berger, T. Benli-Hoppe, L. Peng and E. Wagner:** Hyaluronate siRNA nanoparticles with positive charge display rapid attachment to tumor endothelium and penetration into tumors. *Journal of Controlled Release* 329: 919-933 (2021).
- Mähringer, A., M. Döblinger, M. Henneemann, C. Gruber, D. Fehn, P. I. Scheurle, P. Hosseini, I. Santourian, A. Schirmacher, J. M. Rotter, G. Wittstock, K. Meyer, T. Clark, T. Bein and D. D. Medina:** An Electrically Conducting Three-Dimensional Iron-Catecholate Porous Framework. *Angewandte Chemie-International Edition* 60(33): 18065-18072 (2021).
- Mähringer, A., M. Hennemann, T. Clark, T. Bein and D. D. Medina:** Energy Efficient Ultrahigh Flux Separation of Oily Pollutants from Water with Superhydrophilic Nanoscale Metal-Organic Framework Architectures. *Angewandte Chemie-International Edition* 60(10): 5519-5526 (2021).
- Marczynski, M., K. Jiang, M. Blakeley, V. Srivastava, F. Vilaplana, T. Crouzier and O. Lieleg:** Structural Alterations of Mucins Are Associated with Losses in Functionality. *Biomacromolecules* 22(4): 1600-1613 (2021).
- Marczynski, M. and O. Lieleg:** Forgotten but not gone: Particulate matter as contaminations of mucosal systems. *Biophysics Reviews* 2(3): 031302 (2021).
- Matreux, T., K. Le Vay, A. Schmid, P. Aikkila, L. Belohlavek, A. Z. Caliskanoglu, E. Salibi, A. Kuhnlein, C. Springsklee, B. Scheu, D. B. Dingwell, D. Braun, H. Mutschler and C. B. Mast:** Heat flows in rock cracks naturally optimize salt compositions for ribozymes. *Nature Chemistry* 13(11): 1151-1151 (2021).
- Ochmann, S. E., H. Joshi, E. Büber, H. G. Franquelim, P. Stegemann, B. Sacca, U. F. Keyser, A. Aksimentiev and P. Tinnefeld:** DNA Origami Voltage Sensors for Transmembrane Potentials with Single-Molecule Sensitivity. *Nano Letters* 21(20): 8634-8641 (2021).
- Ochmann, S. E., T. Schröder, C. M. Schulz and P. Tinnefeld:** Quantitative Single-Molecule Measurements of Membrane Charges with DNA Origami Sensors. *Analytical Chemistry* 94(5): 2633-2640 (2022).
- Ploetz, E., G. K. Schuurman-Wolters, N. Zijlstra, A. W. Jager, D. A. Griffith, A. Guskov, G. Gouridis, B. Poolman and T. Cordes:** Structural and biophysical characterization of the tandem substrate-binding domains of the ABC importer GlnPQ. *Open Biology* 11(4) (2021).
- Ramm, B., A. Goychuk, A. Khmelinskaia, P. Blumhardt, H. Eto, K. A. Ganzinger, E. Frey and P. Schwille:** A diffusiophoretic mechanism for ATP-driven transport without motor proteins. *Nature Physics* 17(7): 850 (2021).
- Rosen, M., R. J. Ye, M. Mann, S. Lobe, M. Finsterbusch, O. Guillon and D. Fattakhova-Rohlfing:** Controlling the lithium proton exchange of LLZO to enable reproducible processing and performance optimization. *Journal of Materials Chemistry A* 9(8): 4831-4840 (2021).
- Rosenberger, J. H., T. Goppel, P. W. Kudella, D. Braun, U. Gerland and B. Altaner:** Self-Assembly of Informational Polymers by Templated Ligation. *Physical Review X* 11(3) (2021).
- Savitskiy, S., R. Wachtel, D. Pourjafar-Dehkordi, H. S. Kang, V. Trauschke, D. C. Lamb, M. Sattler, M. Zacharias and A. Itzen:** Proteolysis of Rab32 by Salmonella GtgE induces an inactive GTPase conformation. *Iscience* 24(1) (2021).

* CeNS Publication Award 2021

- Scheurle, P. I., A. Maehringer, A. Biewald, A. Hartschuh, T. Bein and D. D. Medina:** MOF-74(M) Films Obtained through Vapor-Assisted Conversion-Impact on Crystal Orientation and Optical Properties. *Chemistry of Materials* 33(15): 5896-5904 (2021).
- Settele, S., F. J. Berger, S. Lindenthal, S. Zhao, A. A. El Yumin, N. F. Zorn, A. Asyuda, M. Zharnikov, A. Hogege and J. Zaumseil:** Synthetic control over the binding configuration of luminescent sp(3)-defects in single-walled carbon nanotubes. *Nature Communications* 12(1) (2021).
- Silva-Neto, M. L., M. Maldonado, L. D. Menezes, C. B. de Araujo, A. M. Jawaid, R. Busch, A. J. Ritter, R. A. Vaia and A. S. L. Gomes:** Fifth-order optical nonlinear response of semiconducting 2D LTMD MoS₂. *Optics Letters* 46(2): 226-229 (2021).
- Stefancu, A., S. Lee, L. Zhu, M. Liu, R. C. Lucacel, E. Cortes and N. Leopold:** Fermi Level Equilibration at the Metal-Molecule Interface in Plasmonic Systems. *Nano Letters* 21(15): 6592-6599 (2021).
- Stehr, F., J. Stein, J. Bauer, C. Niederauer, R. Jungmann, K. Ganzinger and P. Schwille:** Tracking single particles for hours via continuous DNA-mediated fluorophore exchange. *Nature Communications* 12(1) (2021).
- Stein, J. A. C., A. Ianeselli and D. Braun:** Kinetic Microscale Thermophoresis for Simultaneous Measurement of Binding Affinity and Kinetics. *Angewandte Chemie-International Edition* 60(25): 13988-13995 (2021).
- Swaffer, M. P., J. Kim, D. Chandler-Brown, M. Langhinrichs, G. K. Marinov, W. J. Greenleaf, A. Kundaje, K. M. Schmoller and J. M. Skotheim:** Transcriptional and chromatin-based partitioning mechanisms from cell size. *Molecular Cell* 81(23): 4861 (2021).
- Trenker, S., L. Grunenberg, T. Banerjee, G. Savasci, L. M. Poller, K. I. M. Muggli, F. Haase, C. Ochsenfeld and B. V. Lotsch:** A flavin-inspired covalent organic framework for photocatalytic alcohol oxidation. *Chemical Science* 12(45): 15143-15150 (2021).
- Trixler, F.:** Origin of Nucleic Acids. *Prebiotic Chemistry and the Origin of Life*. A. Neubeck and S. McMahon. Cham, Springer International Publishing: 117-137 (2021).
- Trofymchuk, K., V. Glembockyte, L. Grabenhorst, F. Steiner, C. Vietz, C. Close, M. Pfeiffer, L. Richter, M. L. Schutte, F. Selbach, R. Yaadav, J. Zahringer, Q. S. Wei, A. Ozcan, B. Lalkens, G. P. Acuna and P. Tinnefeld:** Addressable nanoantennas with cleared hotspots for single-molecule detection on a portable smartphone microscope. *Nature Communications* 12(1) (2021).
- Vadia, S., J. Scherzer, H. Thierschmann, C. Schafermeier, C. Dal Savio, T. Taniguchi, K. Watanabe, D. Hunger, K. Karrai and A. Högele:** Open-Cavity in Closed-Cycle Cryostat as a Quantum Optics Platform. *Prx Quantum* 2(4) (2021).
- von der Esch, B., L. D. M. Peters, L. Sauerland and C. Ochsenfeld:** Quantitative Comparison of Experimental and Computed IR-Spectra Extracted from Ab Initio Molecular Dynamics. *Journal of Chemical Theory and Computation* 17(2): 985-995 (2021).
- von Schirnding, C., I. Giopanou, A. Hermawan, L. Wehl, G. Ntaliarda, B. Illes, S. Datz, F. Geisslinger, K. Bartel, A. K. Sommer, M. Lianou, V. Weiss, J. Feckl, A. M. Vollmar, C. Brauchle, G. T. Stathopoulos, E. Wagner, A. Roidl, T. Bein and H. Engelke:** Synergistic Combination of Calcium and Citrate in Mesoporous Nanoparticles Targets Pleural Tumors. *Chem* 7(2): 480-494 (2021).
- von Voithenberg, L. V., A. Barth, V. Trauschke, B. Demarco, S. Tyagi, C. Koehler, E. A. Lemke and D. C. Lamb:** Comparative analysis of the coordinated motion of Hsp70s from different organelles observed by single-molecule three-color FRET. *Proceedings of the National Academy of Sciences of the United States of America* 118(33) (2021).

- Wagner, J., D. Gossl, N. Ustyanovska, M. Y. Xiong, D. Hauser, O. Zhuzhgova, S. Hocevar, B. Taskoparan, L. Poller, S. Datz, H. Engelke, Y. Daali, T. Bein and C. Bourquin:** Mesoporous Silica Nanoparticles as pH-Responsive Carrier for the Immune-Activating Drug Resiquimod Enhance the Local Immune Response in Mice. *ACS Nano* 15(3): 4450-4466 (2021).
- Wang, J., J. Kuhne, T. Karamanos, C. Rockstuhl, S. A. Maier and A. Tittl:** All-Dielectric Crescent Metasurface Sensor Driven by Bound States in the Continuum. *Advanced Functional Materials* 31(46) (2021).
- Wang, X., C. X. Liu, C. C. Gao, K. L. Yao, S. S. M. Masouleh, R. Berte, H. R. Ren, L. D. Menezes, E. Cortes, I. C. Bicket, H. Y. Wang, N. Li, Z. L. Zhang, M. Li, W. Xie, Y. F. Yu, Y. R. Fang, S. P. Zhang, H. X. Xu, A. Vomiero, Y. C. Liu, G. A. Botton, S. A. Maier and H. Y. Liang:** Self-Constructed Multiple Plasmonic Hotspots on an Individual Fractal to Amplify Broadband Hot Electron Generation. *ACS Nano* 15(6): 10553-10564 (2021).
- Zhang, H. Y., J. Bussmann, F. H. Huhnke, J. Devoldere, A. K. Minnaert, W. Jiskoot, F. Serwane, J. Spatz, M. Roding, S. C. De Smedt, K. Braeckmans and K. Remaut:** Together is Better: mRNA Co-Encapsulation in Lipoplexes is Required to Obtain Ratiometric Co-Delivery and Protein Expression on the Single Cell Level. *Advanced Science* 9(4) (2022).
- Zhu, C. B., C. H. Fan, E. Cortes and W. Xie:** In situ surface-enhanced Raman spectroelectrochemistry reveals the molecular conformation of electrolyte additives in Li-ion batteries. *Journal of Materials Chemistry A* 9(35): 20024-20031 (2021).
- Zoller, F., S. Häringer, D. Bohm, H. Illner, M. Doblinger, Z. Sofer, M. Finsterbusch, T. Bein and D. Fattakhova-Rohlfing:** Overcoming the Challenges of Freestanding Tin Oxide-Based Composite Anodes to Achieve High Capacity and Increased Cycling Stability. *Advanced Functional Materials* 31(43) (2021).
- Zoller, F., S. Häringer, D. Bohm, J. Luxa, Z. Sofer and D. Fattakhova-Rohlfing:** Carbonaceous Oxygen Evolution Reaction Catalysts: From Defect and Doping-Induced Activity over Hybrid Compounds to Ordered Framework Structures. *Small* 17(48) (2021).

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