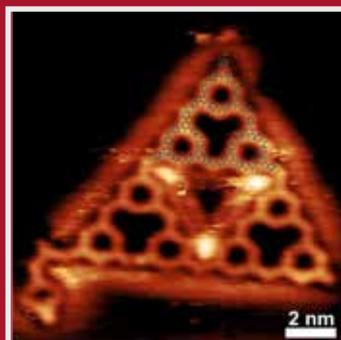
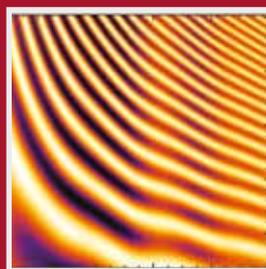
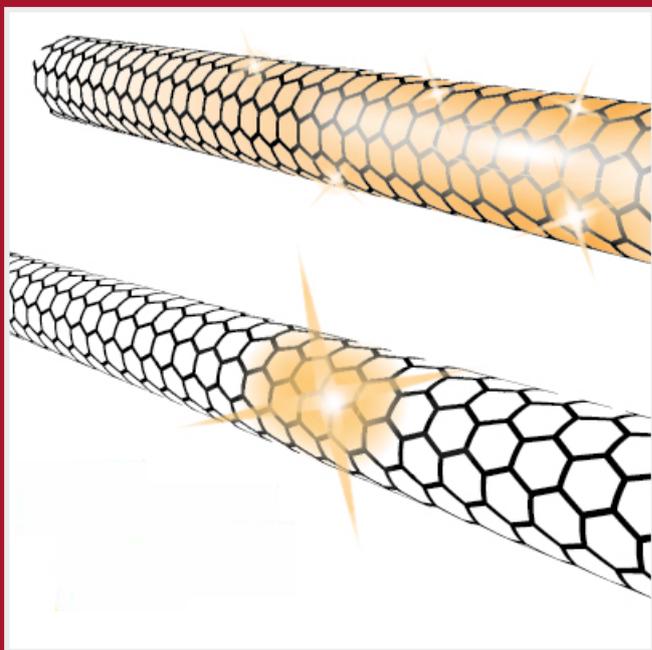


# CENTER FOR NANOSCIENCE ANNUAL REPORT 2016



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## WELCOME



Nanoscience in Munich continues to expand its scope to other disciplines and to explore novel connections at the nanoscale. For example, four new excellence initiative preproposals have grown out of the CeNS-initiated Nanosystems Initiative

Munich (NIM) cluster – Quantum Science and Technology with solid state physics, Bidesign with Biochemistry, Cell ID with Biology, and Origins with Astrophysics.

Nanoscience within NIM has grown so much that a single cluster was no longer sufficient to host the diverse directions. This positive development is facilitated by the fertile breeding grounds provided by the collaborative structures of Munich Nanosciences that are constantly reshaping and diversifying into new fields and thus enabling new research directions. Similarly, the cross-disciplinary graduate schools, such as Quantitative Biosciences Munich, were the initiators for new directions and connections.

The SFB1032 "Nanoagents" was extended - and a new preapplication is in progress: "Recreating the Emergence of Life" is the ambitious title to tackle the origins of life experimentally, merging non-equilibrium processes at the nanoscale to implement molecular replication with geology and astronomy. The aim is to recreate in experiment how the first cycles of Darwinian evolution of life could have emerged.

The start-ups that originated from CeNS continue to grow – they now have more than 450 employees with NanoTemper, Nanion, ibidi, and attocube taking the lead, demonstrating how cross-disciplinary ideas in nanoscience have the best potential for opening up new market possibilities.

The connections between physics and chemistry are reinforced by the newly appointed Oliver Trapp (W3 Chemistry) who is part of the Origins and SFB initiative. And the search for candidates to continue the cross-disciplinary legacy of Bräuchle is making progress. We are grateful for this.

We warmly welcome our new CeNS member Prof. Rasmus Linser and the new extraordinary members Prof. Gregor Cevc, Dr. Anna Cattani-Scholz, Dr. Oliver Thorn-Seshold, and Dr. Christoph Westerhausen. We hope that many new connections will be made!

Central to the approach of CeNS, which aims to facilitate interaction with and among PhD students, are the student representatives, who have been very active in 2016. They organized many events, such as inviting speakers (Prof. Javier Garcia de Abajo, ICFO Barcelona and Prof. Christoph Schmidt, Göttingen), visits to the CeNS start-ups attocube and NanoTemper, a CeNS lab tour in Großhadern, a very nice welcome event for new CeNS students, "Science in a nutshell", and the well-received CadU party.

Last year we introduced a new format for brainstorming and discussing key challenges - we started with "Key challenges in biophysics" and we are looking forward to meet again soon for more such events after an intensive period of proposal writing. We again thank the PIs who organized workshops where CeNS was a cosponsor, such as the 22nd International Conference "DNA Computing and Molecular Programming" with local organizers Tim Liedl, Fritz Simmel, Hendrik Dietz and Ralf Jungmann; the SPIDER/Scipion Workshop organized by Claudia Veigel and Dario Saczko-Brack; and the 5th European Workshop "Advanced Fluorescence Methods" by Don Lamb.

We hope you enjoy reading about the progress made at CeNS, new awards given to CeNS members, our publication prizes, and of course the many very interesting papers.

Finally, we thank the highly professional CeNS management team, Susanne Hennig (managing director), Claudia Leonhardt (team assistant), and Cathleen Hendrich (student assistant) for their great enthusiasm, commitment, and continuous support without which none of the above would have been possible.

*Prof. Dieter Braun*

Member of the Scientific Board of CeNS

## NEW MEMBERS

### DR. ANNA CATTANI-SCHOLZ TU München



Dr. Anna Cattani-Scholz studied organic chemistry at the University "La Sapienza" in Rome and she completed her Ph.D. studies at the TU Munich. After a post-doctoral period in the group of Prof. Oesterhelt at the Max Planck Institut of Biochemistry in Munich, in 2005 she

joined the Walter Schottky Institut at the TUM, where she is completing her habilitation in the physics department in the group of Prof. Stutzmann. Her research is highly multidisciplinary and focuses on the development of new semiconductor hybrid systems towards the optimization of nanodevices, in particular with respect to applications in biosensing.

### PROF. GREGOR CEVC



Gregor Cevc, PhD, MSci, DiplIng, holds advanced degrees in biophysics and biochemistry. Born and educated as a physicist in Slovenia, he continued his professional career in Germany, starting at the Max-Planck Institute for Biophysical Chemistry in Göttingen and

continuing at universities in Essen and Munich. At the Medical Faculty of TU Munich, he set up the Medical Biophysics Laboratory (1988) and served there as a Professor (1988-2000) in the same field.

As one of the national biotechnology pioneers, he founded IDEA AG in Munich, Germany (1993), and spear headed the design and development of its products, including the first independent German biotech product marketing authorization in Switzerland in 2006. At the helm of IDEA (full-time CEO: 1998-2010) he was also jointly responsible for the company financing, R&D and business development, including negotiating and signing the then biggest biotech deal in Germany. More recently, Gregor started further ventures, including the R&D oriented Advanced Treatments Institute network. He has written or edited 3 scientific books and over 200 publications (h-index: 53 / g-index: 114). He was or is an Editorial Board member of several international scientific journals, and a peer-reviewer for over 30 international professional periodicals and over half a dozen research-funding organizations. Gregor was also an Advisory Board Member of the Tel Aviv University and is a Board Member of the University of Nova Gorica.

### PROF. RASMUS LINSER LMU Munich



Prof. Dr. Rasmus Linser studied Chemistry at the University of Göttingen and the Universidad Autónoma de Madrid. He performed his PhD work in the group of Prof. Dr. Bernd Reif at the Leibniz Institute for Molecular Pharmacology (FMP) in Berlin and was awarded a PhD degree by the

Humboldt University Berlin in 2010. He became a research associate and lecturer at the University of New South Wales (UNSW) in Sydney and, financed by a Discovery Early Career Research Award

(DECRA), performed research in the lab of Prof. Dr. Gerhard Wagner at Harvard Medical School, Boston. In 2014, he returned to Göttingen as a junior group leader for solid-state NMR at the Max Planck Institute for Biophysical Chemistry, funded by the Liebig (Verband der Chemischen Industrie) and Emmy Noether (DFG) programs. Rasmus Linser was awarded the Felix Bloch Lecture for excellence in NMR spectroscopy in 2015 (Gesellschaft Deutscher Chemiker, GDCh). He was appointed as a W2 professor for NMR spectroscopy at the LMU and moved with his group to Munich in autumn 2016. The group's research focus is the application of solution and solid-state NMR in a biochemistry context.

## DR. OLIVER THORN-SESHOLD

LMU Munich



Dr. Oliver Thorn-Seshold studied organic and physical chemistry at the University of Sydney and the Ecole Normale Supérieure de Lyon. He was awarded his PhD from the Ecole Normale Supérieure de Lyon in 2013 for chemical biology research into probes for cancer

diagnosis, in the group of Prof. Jens Hasserodt. After a postdoctoral period in the group of Prof. Dirk Trauner at LMU Munich developing light-switchable anticancer compounds, Dr. Thorn-Seshold has been a junior group leader in chemical biology for cancer therapy at LMU since July 2016.

## DR. CHRISTOPH WESTERHAUSEN

University of Augsburg



Dr. Christoph Westerhausen earned a diploma in physics with a specialization in magneto-optical materials and biological physics and took the Bavarian state examination for mathematics and physics teachers in 2008. Between 2009 and 2012 he worked at

the University of Augsburg, the University Hospital in Mannheim, and Boston University in the groups of Prof. S. Schneider and Prof. M. Schneider and received his PhD from the University of Augsburg in 2012. As a project leader in the industrial environment of 'Woelfel Engineering' in Höchberg, he worked in the field of applied acoustics, in room and building acoustics, and investigated the infrasound emissions of wind turbines.

Returning to academia in 2014, he started a junior research group in the lab of Prof. A. Wixforth at the University of Augsburg. Christoph has received national and international funding from the German Research Foundation, the Bavaria California Technology Center, the EU in the framework of a Marie Skłodowska-Curie Actions Innovative Training Network, and other sources. His research group works at the interface of physics, biology and medicine and focuses on the physics of cellular interaction *in vitro* and using model systems. Current projects include systems of lipid membranes interacting with external force fields, nanoparticles or enzymes, cell-substrate and cell-cell interaction for novel biomedical applications, and cell stimulation and creation of cellular networks on a chip. For this purpose, he and his group develop hybrid systems employing surface acoustic waves.

## MEMBERS' NEWS

### CALLS & APPOINTMENTS



**Prof. Ralf Jungmann** (LMU and MPI of Biochemistry) was appointed as a W2 professor at LMU Munich.



**Prof. Bettina Lotsch** (LMU and MPI for Solid State Research) accepted a position as director of the Max Planck Institute for Solid State Research in Stuttgart.



**Prof. Marc Tornow** (TUM) was appointed cooperative department head at the Fraunhofer Research Institution for Microsystems and Solid State Technologies (EMFT), Munich.



**Prof. Dirk Trauner** (LMU) was appointed as a professor at the Department of Chemistry at New York University in the fall of 2016.



**Dr. Stefan Wuttke** (LMU) accepted an offer from the University of Lincoln (UK) as a Senior Lecturer.

### AWARDS



**Prof. Andreas Bausch** (TUM) received an ERC Proof of Concept Grant for his project "Self Organization in Cytoskeletal Systems".



**Dieter Braun** (LMU) was awarded a "CAS Research Group 2016" at the LMU Center for Advanced Studies.



**Prof. Thomas Carell** (LMU) won the Inhoffen Medal 2016.



**Prof. Hendrik Dietz** (TUM) received an ERC Consolidator Grant 2016 for his research on "DNA Origami Motors".



**Prof. Peter Hänggi** (Augsburg University) received an honorary doctorate from Lobachevsky University, Nizhny Novgorod in Russia.



**Prof. Michael Nash** (University of Basel/ETH Zürich, formerly LMU) was awarded an ERC Starting Grant for his project "Molecular Mechanical Adhesives".



**Prof. Christian Ochsenfeld** (LMU) received the "Preis für gute Lehre an Bayerns Universitäten 2016".



**Prof. Petra Schwill** (MPI of Biochemistry) became a Fellow of the Biophysical Society.



**Prof. Fritz Simmel** (TUM) won the Rozenberg Tulip Award in DNA Computing.



**Prof. Dirk Trauner** (LMU) received the Emil Fischer Medal 2016 from the GDCh and the Otto-Bayer-Preis 2016 from the Bayer Science & Education Foundation.



**Dr. Alexander Urban** (LMU) was awarded an LMUexcellent Junior Researcher Grant.

## COLLABORATIVE RESEARCH PROJECTS

The collaborative research center **SFB1032 "Nanoagents for the spatiotemporal control of molecular and cellular reactions"** receives funding for a 2nd period of another four years from July 2016 – June 2020. Twenty PIs, thereof nineteen CeNS members, will continue their joint efforts on designing and studying synthetic biomolecular constructs, nanoagents, which fulfil biomimetic or entirely novel functions. The SFB combines physical and chemical approaches for the assembly and positioning of biological molecules, develops nanotechnology methods to follow molecular processes at the nanoscale over time and comprises theoretical modelling from the molecular to the mesoscopic scale.

■ [sfb1032.physik.uni-muenchen.de](http://sfb1032.physik.uni-muenchen.de)

The Bavarian-based research network "**Solar Technologies Go Hybrid**", in short **SolTech**, in which five Bavarian universities are collaborating to develop novel material systems for solar energy conversion, will be funded with a total amount of 17 million Euros for an additional five years by the Free State of Bavaria. This unique consortium began its collaborative research activities in 2012 as an action within the framework of the "Energy Transition". After a recent evaluation, the SolTech network, including eight CeNS members, can now continue its collaborative research work to add solutions to one of the most important global challenges.

■ [www.soltech-go-hybrid.de](http://www.soltech-go-hybrid.de)

The collaborative research center **SFB1035 "Control of protein function by conformational switching"**, with two CeNS members involved, successfully passed the 2nd funding round of another four years. The SFB 1035 aims at understanding the principles that allow regulation of protein function by structural transitions between different protein conformations.

■ [www.sfb1035.tum.de](http://www.sfb1035.tum.de)

## CENS AWARDS

### CENS TRAVEL AWARDS

In 2016, thirteen CeNS PhD students and one postdoc won CeNS travel awards to present their work at international conferences and workshops such as the MRS Spring and Fall meeting, the Gordon Research Conference, or the Biophysical Society Meeting. The recipients of the awards selected by the CeNS board came from nine different CeNS groups, from the Department of Chemistry and the Department of Physics. Examples of three award winners illustrate their contributions.



During her stay at the **MOF 2016 conference**, the largest and most renowned conference in the field of Metal Organic Frameworks and open framework compounds, **Laura Ascherl** (Prof. Thomas Bein's group) presented the latest results of her research in the course of a poster session. Her poster focused on a concept for realizing highly crystalline covalent organic frameworks by making use of the unique three-dimensional conformation of the building blocks. The poster was highly frequented by various researchers, which allowed Laura to make contact with a lot of prospective collaboration partners. Laura won third prize for her poster.

**Ascherl, L.**, Sick, T., Margraf, J. T., Lapidus, S. H., Calik, M., Hettstedt, C., Karaghiosoff, K., Döblinger, M., Clark, T., Chapman, K. W., Auras, F., Bein, T.: Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks; *Nature Chem.* **8**, 310-316 (2016).



**Thomas Simon**, on of Prof. Jochen Feldmann's PhD students, presented recent results about strong coupling between plasmons and excitons at the **SPIE optics&photonics conference** in San Diego on August 31st. The contribu-

tion was a collaboration between the Chair for Photonics and Optoelectronics and the groups of Prof. Liz-Marzan and Prof. Rakovich from San Sebastian. Gold nanorods coated with a J-aggregated cyanine dye were used to obtain coupled hybrid resonances, so-called "plexcitons". By applying ultrafast spectroscopy, they were able to demonstrate that plexcitons show both plasmonic and excitonic behavior. Their nature can be tuned by varying the spectral overlap between the plasmon of the gold nanorod and the exciton of the dye molecules.

**T. Simon**, D. Melnikau, A. Sánchez-Iglesias, M. Grzelczak, L. M. Liz-Marzan, Y. P. Rakovich, J. Feldmann and A. S. Urban: Exploring the Optical Nonlinearities of Plasmon-Exciton Hybrid Resonances in Coupled Colloidal Nanostructures; *The Journal of Physical Chemistry C*, **120** (22), 12226-12233 (2016).



The oral presentation given by **Harald Budde** (Prof. Achim Hartschuh's group) at the **E-MRS Spring Meeting** in Lille (France) entitled Raman Radiation Patterns of Graphene was based on a recently published report.

Basics about radiation patterns in general as well as polarization-dependent Raman spectroscopy of graphene were introduced. The talk focused on the extrinsic effect of depolarization present for polarized emission gathered with a high numerical aperture microscope objective. Depolarization is the origin of the dependence of the Raman 2D polarization ratio and the 2D / G intensity ratio on the collection angle. Finally, an equation was developed, taking depolarization into consideration.

**Budde H.**, Coca-López N., Shi X., Ciesielski R., Lombardo A., Yoon D., Ferrari A.C., Hartschuh A.: Raman Radiation Patterns of Graphene; *ACS Nano*, doi: 10.1021/acsnano.5b06631 (2016).

■ [www.cens.de/research/cens-travel-award/](http://www.cens.de/research/cens-travel-award/)

## CENS PUBLICATION AWARDS

On November 25, the winners of the 2016 CeNS Publication Awards were announced to the CeNS members during a celebratory event. This award recognized remarkably successful cooperation projects within CeNS as well as outstanding research by individual research groups from CeNS.

### "Best Interdisciplinary Publication":

- J. A. Frank, H. G. Franquelim, **Petra Schwille and Dirk Trauner**: Optical Control of Lipid Rafts with Photoswitchable Ceramides; *JACS*, see p. 42
- D. J. Lee, E. Kessel, D. Edinger, D. He, P. M. Klein, L. V. von Voithenberg, **Don C. Lamb**, U. Lächelt, T. Lehto and **Ernst Wagner**: Dual antitumor potency of EG5 siRNA nanoplexes armed with cytotoxic bifunctional glutamyl-methotrexate targeting ligand; *Biomaterials*, see p. 45
- E. M. Roller, C. Argyropoulos, **Alexander Högele, Tim Liedl** and M. Pilo-Pais: Plasmon-Exciton Coupling Using DNA Templates; *Nano Letters*, see p. 29

### "Scientific Breakthrough":

- J. P. Müller, S. Mielke, A. Löf, T. Obser, C. Beer, L. K. Bruetzl, D. A. Pippig, W. Vanderlinden, **Jan Lipfert**, R. Schneppenheim and **Martin Benoit**: Force sensing by the vascular protein von Willebrand factor is tuned by a strong intermonomer interaction; *PNAS*, see p. 22
- J. Denk, L. Huber, E. Reithmann and **Erwin Frey**: Active Curved Polymers Form Vortex Patterns on Membranes; *PRL*, see p. 25
- V. S. Vyas, F. Haase, L. Stegbauer, G. Savasci, F. Podjaski, **Christian Ochsenfeld** and **Bettina V. Lotsch**: A tunable azine covalent organic framework platform for visible light-induced hydrogen generation; *Nature Communications*, see *CeNS Annual Report 2015*
- L. Ascherl, T. Sick, J. T. Margraf, S. H. Lapidus, M. Calik, C. Hettstedt, K. Karaghiosoff, M. Döblinger, T. Clark, K. W. Chapman, F. Auras and **Thomas Bein**: Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks; *Nature Chemistry*, see p. 20

### "Best Junior Scientist Publication":

- M. Morasch, **Dieter Braun** and **Christof B. Mast**: Heat-Flow-Driven Oligonucleotide Gelation Separates Single-Base Differences; *Angew. Ch. Int. Ed.*, see p. 21
  - A. Babynina, M. Fedoruk, P. Kuhler, A. Meledin, M. Döblinger and **Theobald Lohmüller**: Bending Gold Nanorods with Light; *Nano Letters*, see p. 36
  - V. A. Hintermayr, A. F. Richter, F. Ehrat, M. Döblinger, W. Vanderlinden, J. A. Sichert, Y. Tong, L. Polavarapu, **Jochen Feldmann** and **Alexander S. Urban**: Tuning the Optical Properties of Perovskite Nanoplatelets through Composition and Thickness by Ligand-Assisted Exfoliation; *Advanced Materials*, see p. 43
- [www.cens.de/research/cens-publication-award](http://www.cens.de/research/cens-publication-award)



Jan Lipfert, Achim Löf, Martin Benoit and Linda Brützel were among the proud winners of a CeNS publication award in the category "Scientific breakthrough".



The CeNS band "UnCeNSiert" at the CadU.

## SPIN-OFF NEWS

### ATTOCUBE

Since April 1, 2016 attocube has a new management board: After 15 successful years with double-digit growth rates, CeNS members Dr. Dirk Haft and Professor Khaled Karraï transferred the running of the company to Dr. Martin Zech. Alongside his new function on the Management Board of WITTENSTEIN AG, Dirk Haft continues as Chairman of the Supervisory Board, and Khaled Karraï continues to support the company as Scientific Director, steering the development of ideas as Innovation Manager and accompanying the development processes for new products as Scientific Mentor.



Khaled Karraï (third from right) and Dirk Haft (fourth from right) at the groundbreaking ceremony for attocube's new headquarter.



Image of the future attocube systems headquarter (Renderings: HENN Architekten).

In addition to the executive staff changes, attocube will move its headquarters to Haar in 2018, where a new 9,175 m<sup>2</sup> building is currently being erected. "The new building offers the chance to construct it according to our requirements and to redefine current modes of operation, thereby creating a place that will represent attocube and allow our employees to identify with it", says Dr. Zech.

■ [www.attocube.com](http://www.attocube.com)



### NANOTEMPER TECHNOLOGIES

FOCUS and Statista have ranked NanoTemper Technologies among the 500 fastest-growing companies in Germany. They identified companies with exceptional growth rates between 2012 and 2015 as "Growth Champions 2017". NanoTemper Technologies ranked # 2 in the "Chemistry and Pharma" category, with a growth rate of 65% per year.

■ [nanotempertech.com](http://nanotempertech.com)



Students discussing with Philipp Baaske at the CeNS company visit at Nanotemper's headquarter in October 2016.

## IBIDI

With their innovative, joint project "ibidi–Analysis of Living Cells", ibidi GmbH became a top finalist in the German nation wide competition, "Deutschland: Land der Ideen 2016" (Germany, Land of Ideas 2016). The 2016 contest goal was to find and reward companies and organizations that create value by working with others, and ibidi teamed up with various partners to expand their knowledge of live cell imaging techniques.

In 2015, ibidi developed the  $\mu$ -Slide CorrSight™ Live, the product that earned the award, which correlates the molecular specificity of light microscopy with the high structural resolution of electron microscopy. This finally makes it possible to accurately visualize cell and tissue structures with both techniques.



Valentin Kahl (second from left) and Roman Zantl (third from left) receiving the ibidi's award "Landmark 2016".

ibidi also received a distinguished "FINALIST" INDUSTRIEPREIS 2016, in the biotechnology category, for their unique  $\mu$ -Slide Membrane ibiPore Flow—a product designed for migration and transport studies on cells. This is the second time since 2012 that ibidi has been awarded this honor.

■ [www.ibidi.de](http://www.ibidi.de)



## NEASPEC

Neaspec's neaSNOM microscope won the prestigious iF design award 2016 in the category "products". Every year iF International Forum Design GmbH recognizes particularly well-designed industrial products to communicate the importance of design. The neaSNOM near-field microscope was among the winners because it opens the view to nanoscale analysis in material sciences, chemistry, polymer sciences, and even life sciences by spectroscopy. The complex inner structure with highly precise optical assemblies is structured to a set of modules that can be arranged according to individual customers' demands. The modularity allows flexibility to add different laser sources and the illustration of the beam path explains which settings apply to the measurement.

■ [www.neaspec.com](http://www.neaspec.com)



## EVENTS & ACTIVITIES

### FOCUS WORKSHOPS

The **22nd International Conference on DNA Computing and Molecular Programming** was organized under the auspices of the International Society for Nanoscale Science, Computation and Engineering (ISNSCE) by CeNS members Tim Liedl, Fritz Simmel, Hendrik Dietz, and Ralf Jungmann. The conference took place in Munich on September 4-6, 2016 and provided a premier forum where scientists from diverse backgrounds came together with the common purpose of applying principles and tools of computer science, physics, chemistry and mathematics to advance molecular-scale engineering and biology.



On September 14, fifteen CeNS members gathered at the Internationales Begegnungszentrum (IBZ) for a **workshop entitled “Key challenges in biophysics”**. Dieter Braun, Erwin Frey, Tim Liedl and Claudia Veigel presented hot topics and challenges of the field, followed by lively discussions among the participants.

Dario Saczko-Brack and Claudia Veigel organized a **SPIDER & Scipion Workshop on Image-processing of electron micrographs** on November 3-4, 2016. Participants received hands-on software training for single particle analysis from leading experts. In addition, three guest speakers presented their research in the field of electron microscopy.

The **5th European Workshop on Advanced Fluorescence Methods** took place on December 5-9, 2016 at LMU Munich. Organized by Don Lamb and

supported by CeNS, the workshop consisted of advanced theoretical lectures by experts in the field and computer-based training on data analysis and simulations, underscoring what was taught during the lectures. The theoretical part was complemented by hands-on laboratory training using the fluorescence microscopy instrumentation of the LMU.

■ [www.cens.de/calendar/past-workshops-events](http://www.cens.de/calendar/past-workshops-events)

### 2016 CeNS WORKSHOP VENICE

The 2016 CeNS Workshop in Venice explored the nanoscale under the title “Nanoscale Matter – Novel Concepts and Functions”. About 90 CeNS members gathered once again on the beautiful island of San Servolo to learn from and hold discussions with 26 invited international scientists. The program committee (Hanna Engelke, Alexander Högele, Ralf Jungmann, Matthias Punk, Marc Tornow, and Thomas Weitz) had put together a truly interdisciplinary program, including single-molecule electronics, super-resolution microscopy, charge transport in nanomaterials, and topological insulators. During two poster sessions, the CeNS students had the opportunity to discuss their research with invited speakers and CeNS members. In addition, two young CeNS scientists, Daniela Ziegler and Florian Schüder, presented their work in short talks.

■ [www.cens.de/calendar/workshops-events/venice-2016](http://www.cens.de/calendar/workshops-events/venice-2016)



## INDUSTRY AND TECHNOLOGY TRANSFER

In 2016, CeNS arranged a number of events to promote interactions with CeNS spin-offs and other partners from industry, and to give junior scientists an overview of career paths outside academia.

As a joint event with the European Patent Academy (EPA) and patent attorney Dr. Stefan R. Huebner, CeNS organized a two-day workshop **"Patents – how to protect your ideas"**. In the first part, participants learned about various aspects of patent applications and the patenting procedure at the EPO. In the following interactive part, participants put themselves into the roles of patent attorneys and judges. They worked on a real patent infringement case and finally presented their arguments in a lively mock trial. A discussion of career opportunities in the IP sector completed the program.



On the initiative of the CeNS student representatives, CeNS organized several **on-site company visits**. In June 2016, a student group had the unique opportunity to visit **attocube systems'** R&D and production site in Königinstraße. Khaled Karraï, founder and CEO of attocube and CeNS member, provided fascinating insights into attocube's history, product lines, and visions. In addition, the students had the chance to discuss future career and business opportunities.

In November, a group of PhD students visited the CeNS spin-off **NanoTemper Technologies** in the Werkstadt Sendling. CeNS member Philipp Baaske, founder and CEO of NanoTemper Technologies, made time for the CENS group and talked about the company's foundation and latest developments. The students were able to take a look at R&D facilities, production, and offices.

The third company visit was to **Roche Penzberg**, a global player located in the Munich area. The 15 participants were informed about early development in Diagnostic Research and career opportunities for physicists and chemists.



The annual event **"CeNS meets industry"** provided insights into various career options outside academia. CeNS alumna Dr. Halina Dunn (AG Bein) opened with a presentation of a patent examiner's work at the EPO. Her talk was followed by Dr. Svenja Lippok (alumna of AG Rädler) who gave an introduction to "Tissue Phenomics", i.e. image analysis and data mining for the analysis of cancer cells, at Definiens AG. Dr. Tobias Roesener, Instrument Systems GmbH, spoke about high-quality systems for the precise measurement of LEDs and LED modules.

In a fascinating talk, Dr. Jürgen Scriba (alumnus of AG Kotthaus) connected physics, science journalism, media art and organ building and demonstrated that physicists are truly versatile experts. Last but not least, Dr. Antonio Manetto (alumnus of AG Carell) presented the spin-off baseclick GmbH and shared his experiences in starting a company.

■ [www.cens.de/calendar/past-workshops-events](http://www.cens.de/calendar/past-workshops-events)



## EVENTS & ACTIVITIES

### CAREER EVENTS AND KEY QUALIFICATION WORKSHOPS

CeNS supported its junior researchers on their way to becoming independent scientists with three special events. The workshop **"How to start my own group"** was aimed at junior group leaders and postdocs and gave them the opportunity to look into their new role and various aspects of group management. In her talk **"Avoiding and Recovering from Common Postdoc Mistakes"**, science journalist Alaina G. Levine shared her experiences with the CeNS students. The workshop **"Leading and supervising in science"** addressed advanced PhD students and postdocs and dealt with supervising Bachelor and Master students in the lab effectively.

In the workshop **"Optimizing writing strategies for getting published in English"** CeNS PhD students expanded their writing skills and worked on their own texts.

■ [www.cens.de/calendar/past-workshops-events](http://www.cens.de/calendar/past-workshops-events)



### CeNS LAB TOUR

The CeNS 2016 lab tour, organized by the student representatives, took place at the Faculty for Chemistry and Pharmacy in Großhadern in July. The participants were guided through the labs of Prof. Hartschuh, Prof. Lotsch, Prof. Gaul, and Prof. Wagner by peer PhD students. They learned about research and infrastructure such as optical imaging and spectroscopy with nanoscale spatial

resolution, nanochemistry, nanomedicine with nucleic acid based therapeutics, and systems biology of gene regulation. The tour was followed by a student-organized barbecue on the campus, a perfect opportunity to meet people from different CeNS groups and to exchange ideas.

■ [www.cens.de/calendar/past-workshops-events](http://www.cens.de/calendar/past-workshops-events)



### CeNS STUDENT REPRESENTATIVES

In March 2016, three new CeNS student representatives were elected by the CeNS associates in an online election: **Nicolás Coca López** studied physics at the UCM (Spain) and the TUM. Currently, he is doing his PhD in Achim Hartschuh's group, focusing on antenna-enhanced microscopy and spectroscopy of graphene. **Isabella Graf** (née Krämer) studied Physics at LMU and spent one year abroad and is now doing her PhD with Erwin Frey within the graduate school QBM. **Ines Trübenbach** studied pharmacy in Freiburg and is in the second year of her PhD at LMU in the group of Ernst Wagner, working on nanoparticulate drug delivery to tumors. Here, they report on their experiences during their time as CeNS student representatives.

#### Why did you stand for election as a CeNS representative?

**Nico:** I really enjoyed the CeNS activities during the previous two years. So I thought that I would



CeNS Student representatives Nicolás Coca López, Isabella Graf and Ines Trübenbach

like to actively contribute to the organization. Plus, I think it is a nice way to meet more people involved in CeNS.

**Isabella:** I think an essential part of CeNS is to promote exchange between PhD students from different groups and to offer various opportunities for students to broaden their horizons (workshops, CeNS meets industry, lab tours etc.). To maintain such activities, it is necessary to have close contact between the students and the management board and it is very important that students get involved and give their input.

#### **What did your work as a student representative involve?**

**Nico:** Our main task was to organize events for the CeNS associates and serve as point of contact for CeNS students. We normally met with Susanne to gather ideas for different events (special seminars, company visits, workshops), and after an online vote by the CeNS associates in which they could choose their preferred options, we would organize the activity.

#### **What activities and events did you plan during your time as student representative?**

**Ines:** We actually planned many activities as a team, like the lab tour in summer and the "Science in a Nutshell" event. I was responsible for the CeNS get-together party in November. The CeNS is really well organized: there are contacts and connections outside the university and lots of experience. That really simplified our work.

#### **Which CeNS event did you personally find most interesting?**

**Isabella:** I think I enjoyed the afternoon with lab tours and the BBQ most. As a theorist I have very rarely been in a lab and it was great to get to see three very different labs and to get to know other PhD students working in Großhadern.

**Nico:** I most enjoyed the two special journal clubs with Prof. Garcia de Abajo and Prof. Schmidt. Having lunch with a small group of students, followed by a journal club, in which the guests discussed their own work, allowed very close interaction. It was very interesting and fruitful, and the lunch prepared by the CeNS management team was delicious!

**Ines:** The event I found most interesting was "CeNS meets industry" last summer. Different career paths were presented by former CeNS members. Especially the talk by Dr. Jürgen Scriba was very unusual and inspiring. The summer party that followed the event was a lot of fun, too.

#### **How does CeNS support its PhD students?**

**Isabella:** CeNS offers a lot of different activities for students to network, to find out what to do after their PhD and to enjoy science in a very relaxed atmosphere. There are possibilities for financial support and maybe most importantly, there are always people that are happy to help, to give advice and that are very open for new suggestions and ideas.

**Ines:** Additionally, CeNS really promotes interdepartmental networking. In a city like Munich, with its different campuses, this is very important. Of course, the monetary support is nice, too: with its Publication Awards and Nano Innovation Award, CeNS values the work of its PhD students and the travel grants give us the opportunity to participate in conferences abroad.

#### **Last but not least, is there anything else you would like to say?**

**Isabella:** I had a great time working with Nico and Ines and we got a lot of help from the CeNS team in implementing our ideas (thank you, Claudia, Marilena, and in particular Susanne!).

**Ines:** I would like to thank Nico, Isabella and Susanne. It was great fun working with them during the last year.

**Nico:** Taking part in the CeNS student representatives team was a very rewarding experience. I really enjoyed working with Ines and Isabella and feel very grateful to Claudia, Marilena, and especially, Susanne. Thank you!

#### **Thank you for the interview!**

■ [www.cens.de/young-academics](http://www.cens.de/young-academics)

## NEW NANO INSTITUTE AT THE FUTURE LMU PHYSICS CAMPUS

On December 6, 2016 the topping-out ceremony for the new LMU Nano Institute near the Englischer Garten was held. From 2019 onwards, the nano institute will be home to Professor Jochen Feldmann's Chair of Photonics and Optoelectronics, and a newly established Chair for Hybrid Nanosystems. The new building will provide laboratories, state-of-the-art clean rooms, offices, common rooms and conference rooms for researchers – and, of course, lots of space for the necessary instrumentation and technology.



Topping-out ceremony in December 2016.

The Nano-Institute is intended to make a major contribution to the infrastructure required to implement the transition to sustainable energy sources (the 'Energiewende') in Germany. The Research Network "Solar Technologies go hybrid" will undertake basic research in the areas of photovoltaics and photocatalysis here. The major aim is



The building will be faced with vertically patterned tiles coated with a special glaze – a clever reference to the significance of surface coatings in the field of nanotechnology. (Source: KKLf Architekten, Berlin)

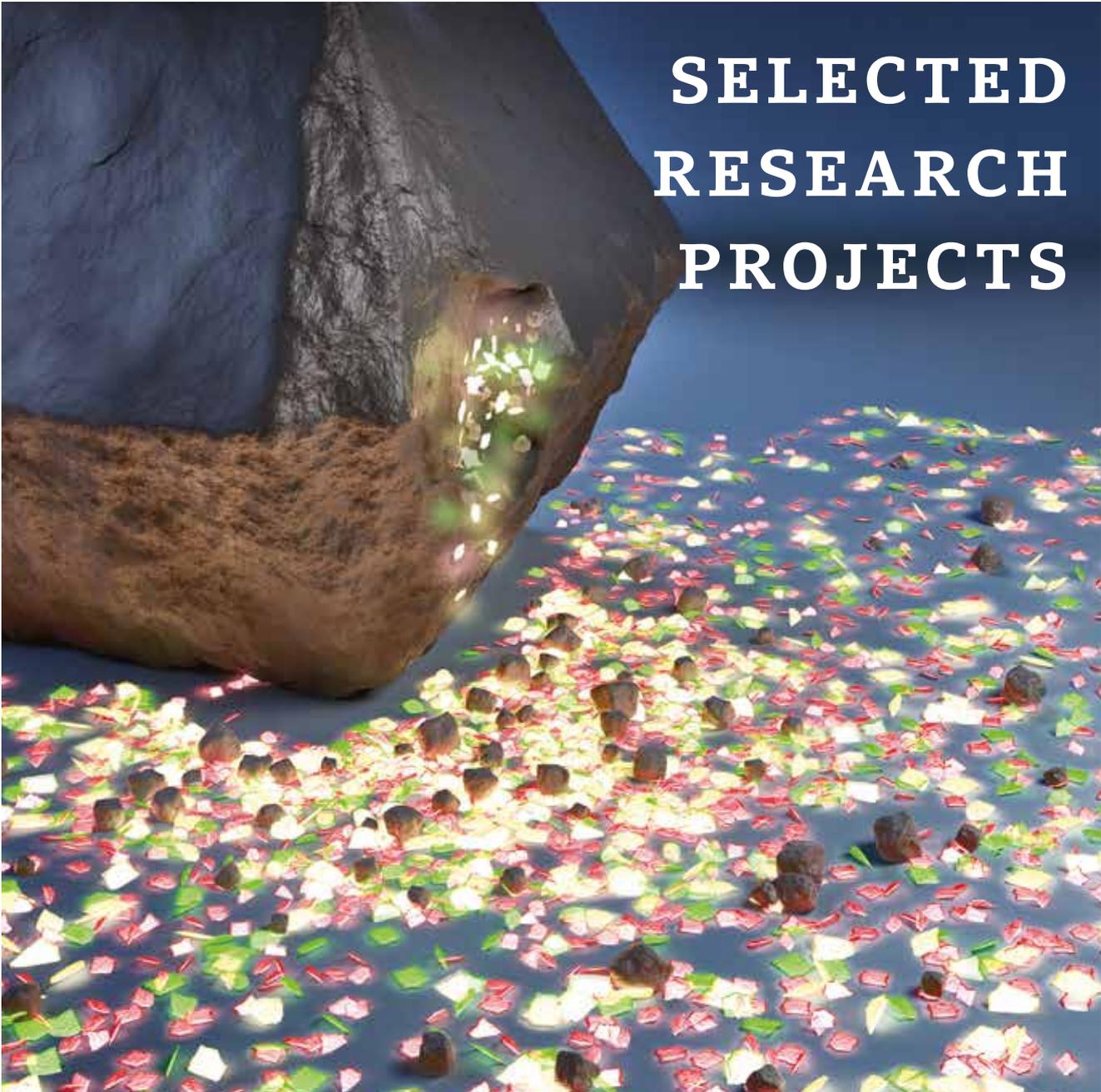
to explore and develop innovative ways of converting solar energy into electricity and non-fossil energy sources. Indeed, the roof of the new building is designed to accommodate a photovoltaic system as well as test-beds for nanotechnology. Construction will be completed in 2018. The estimated cost of the venture is 33.5 million euros.

## CENTER FOR MOLECULAR BIOSYSTEMS (BIOSYSM)

A new center devoted to research on Molecular Biosystems is the 2016 addition to LMU's HighTechCampus in Grosshadern/Martinsried. The new building is located only a short distance from the Gene Center and LMU's Chemistry Institutes. Thematically, the new Center for Molecular Biosystems (BioSysM) fits perfectly into the array of research institutions located on LMU's HighTechCampus in Martinsried/Grosshadern. BioSysM, which accommodates a staff of 200, brings together the research groups at LMU that focus on systems biology, a relatively young discipline which has considerable potential to transform the fields of the life sciences and medicine. The new center for Molecular Biosystems Research houses four established labs, including the group of CeNS member Ulrike Gaul, Professor of Organismic Biochemistry and scientific coordinator of the new center. In addition, four independent junior research groups will complement the scientific portfolio of the center. Finally, CeNS member Don Lamb, Professor of Physical Chemistry, has moved to the new center with part of his group.



The new BioSysM Institute on the HighTechCampus in Grosshadern/Martinsried opened in April 2016.



**SELECTED  
RESEARCH  
PROJECTS**

## SELECTED RESEARCH PROJECTS

- 1 Thomas Bein, Hanna Engelke, Heinrich Leonhardt:** Intracellular chromobody delivery by mesoporous silica nanoparticles for antigen targeting and visualization in real time
- 2 Thomas Bein:** Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks
- 3 Thomas Bein, Achim Hartschuh:** From highly crystalline to outer surface-functionalized covalent organic frameworks – a modulation approach
- 4 Dieter Braun:** Nonequilibrium at the micro-scale: From biotechnology for medicine to unraveling the emergence of life
- 5 Martin Benoit, Jan Lipfert:** A force-sensing protein in the blood flow
- 6 Christoph Bräuchle, Hanna Engelke, Achim Wixforth:** Toxicity of nanoparticles emitted by catalytic converters of automobiles/environmental pollution
- 7 Erwin Frey:** Formation of vortex patterns of active curved polymers on membranes
- 8 Hermann E. Gaub, Michael A. Nash:** Designer cellulosomes
- 9 Achim Hartschuh, Thomas Bein:** Studying and optimizing charge transport in hybrid halid perovskite solar cell materials
- 10 Alexander Högele:** Exciton localization in carbon nanotubes
- 11 Alexander Högele, Tim Liedl:** Plasmon–exciton coupling using DNA templates
- 12 Fritz Keilmann:** Ultrafast optical control of graphene plasmons
- 13 Ulrich Lächelt, Ernst Wagner, Thomas Bein, Stefan Wuttke, Joachim Rädler:** Coordinative self-assembly of His-tagged units with metal–organic frameworks
- 14 Markus Lackinger, Wolfgang M. Heckl:** On-surface synthesis of highly stable molecular Sierpinski triangles
- 15 Don C. Lamb:** Dynamics of the Spliceosome
- 16 Oliver Lieleg:** Hydrophobic properties of biofilm-enriched hybrid mortar
- 17 Jan Lipfert, Hendrik Dietz:** SAXSy DNA origami
- 18 Theobald Lohmüller:** Bending gold nanorods with light
- 19 Bettina V. Lotsch:** Dark photocatalysis with 2D carbon nitrides
- 20 Ralf Metzler:** Protein crowding in lipid bilayers: Non-Gaussian anomalous diffusion
- 21 Bert Nickel, Tim Liedl, Joachim Rädler:** Shape and inner structure of DNA origami in harsh ionic conditions
- 22 Christian Ochsenfeld:** Explaining the NMR spectrum of the active site of photoactive yellow protein as a dynamic equilibrium of hydrogen-bond conformers
- 23 Madeleine Opitz, Oliver Lieleg:** Direct comparison of physical properties of *Bacillus subtilis* NCIB 3610 and B-1 biofilms
- 24 Petra Schwillie, Dirk Trauner:** Control of lipid rafts with photoswitchable ceramides
- 25 Alexander S. Urban, Jochen Feldmann:** Tuning the optical properties of perovskite nanoplatelets through composition and thickness by ligand-assisted exfoliation
- 26 Claudia Veigel:** Mechanics and structure of molecular motor proteins
- 27 Ernst Wagner, Don C. Lamb, Joachim Rädler:** Folate receptor targeted si RNA nanoparticles for tumoral Eglin 5 gene silencing and cure of mice
- 28 Eva Weig, Jörg P. Kotthaus:** Classical Stückelberg interferometry of a nanomechanical two-mode system
- 29 Stefan Wuttke, Don C. Lamb:** Heterogeneities in metal-organic frameworks

## INTRACELLULAR CHROMOBODY DELIVERY BY MESOPOROUS SILICA NANOPARTICLES FOR ANTIGEN TARGETING AND VISUALIZATION IN REAL TIME

Prof. Thomas Bein (LMU München, Chemistry Department)

■ [bein.cup.uni-muenchen.de](http://bein.cup.uni-muenchen.de)

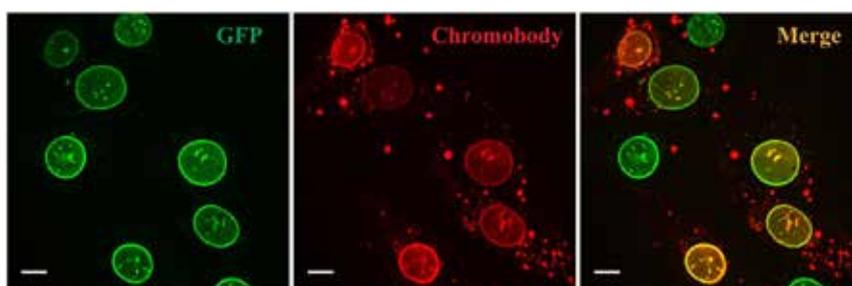
Dr. Hanna Engelke (LMU München, Chemistry Department)

■ [www.cup.lmu.de/pc/engelke/](http://www.cup.lmu.de/pc/engelke/)

Prof. Heinrich Leonhardt (LMU Munich, Department of Biology)

■ [www.bioimaging.bio.lmu.de/research/research-group-leonhardt](http://www.bioimaging.bio.lmu.de/research/research-group-leonhardt)

In this collaboration between the groups of Heinrich Leonhardt and Thomas Bein, the researchers have developed the first example of highly efficient intracellular delivery of chromobodies by nano-carriers (mesoporous silica nanoparticles, MSNs) and visualize the antigen targeting in real time by live cell imaging. The newly synthesized multifunctional large-pore MSNs grafted with metal complexes are promising universal nano-carriers for intracellular his-tagged protein delivery. They also demonstrate quantification of cellular uptake efficiency of MSNs, endosomal release efficiency of chromobodies, and cell toxicity/cell viability after treatment with various endosomal release triggers, using a high content imaging system. Chromobodies, the fluorescent nanobodies, are single-domain antigen-specific small antibodies, which have been used in both basic biological studies and clinical investigations based on their unique biological and pharmacological properties. They are also powerful tools for bio-imaging, especially for illuminating endogenous protein



**Figure 1:** Live cell confocal imaging of intracellular chromobody delivery. 24 h post incubation of MSNs loaded with chromobodies on mouse embryonic fibroblasts (MEFs) expressing EGFP fused to LMNA (an inner nuclear membrane protein). When Atto 647N labeled GFP-specific chromobodies are delivered to and subsequently released from endosomes, they passively diffuse through the nuclear envelope and bind to GFP molecules on the MNA structure of the nucleus. Therefore, a distinct microscopic co-localization signal from EGFP-LMNA and GFP-specific chromobodies can be observed.

structures or biological processes in living cells. By using the above MSNs as nano-carriers the researchers overcome the conventional challenges (low cellular uptake efficiency and endosomal trapping) of protein delivery in live cells. This research combines two powerful nano-tools and provides a new strategy for efficient intracellular chromobody delivery to visualize cellular structures and thus to study biological processes in living cells.

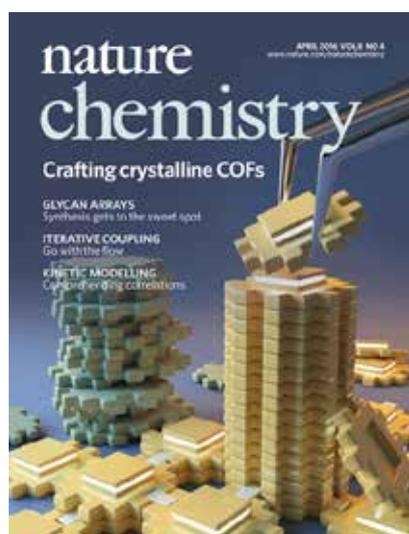
■ **H.-Y. Chiu, W. Deng, H. Engelke, J. Helma, H. Leonhardt, and T. Bein:** *Intracellular chromobody delivery by mesoporous silica nanoparticles for antigen targeting and visualization in real time*; *Sci. Rep.* 6, 25019 (2016)

## MOLECULAR DOCKING SITES DESIGNED FOR THE GENERATION OF HIGHLY CRYSTALLINE COVALENT ORGANIC FRAMEWORKS\*

Prof. Thomas Bein (LMU München, Chemistry Department)

■ [bein.cup.uni-muenchen.de](http://bein.cup.uni-muenchen.de)

Crystalline order in molecular networks can have a profound impact on physical properties,



**Figure 1:** Schematic visualization of the stacking concept developed for the COF materials (Cover graphics, image: Christoph Hohmann, NIM).

including the transport of molecules, charge carriers and electronic excitations. The group of Thomas Bein has developed and successfully applied a new synthetic concept for introducing an exceptionally high degree of crystallinity into covalent organic frameworks (COFs). Using the inherent molecular conformation of rigid, screw-shaped building units to generate self-repeating docking sites, consecutive COF sheets can snap into position during crystal growth. This way, the researchers were able to realise COFs featuring an unmatched degree of crystallinity and well-defined crystal facets. Having demonstrated the generality of this approach for a

number of combinations of different multidentate building blocks and linear bridging units, they expect this strategy to be transferable to a broad range of customised COFs, with significant impact on their physical properties.

■ **L. Ascherl, T. Sick, J. T. Margraf, S. H. Lapidus, M. Calik, C. Hettstedt, K. Karaghiosoff, M. Doeblinger, T. Clark, K. W. Chapman, F. Auras, and T. Bein:** *Molecular docking sites designed for the generation of highly crystalline covalent organic frameworks*; *Nat. Chem.* 8 (4), 310-316 (2016)

## FROM HIGHLY CRYSTALLINE TO OUTER SURFACE-FUNCTIONALIZED COVALENT ORGANIC FRAMEWORKS – A MODULATION APPROACH

Prof. Thomas Bein (LMU München, Chemistry Department)

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Prof. Achim Hartschuh (LMU München, Chemistry Department)

■ [www.cup.uni-muenchen.de/pc/hartschuh](http://www.cup.uni-muenchen.de/pc/hartschuh)

Crystallinity and porosity are of central importance for many properties of covalent organic frameworks (COFs) including adsorption, diffusion and elec-

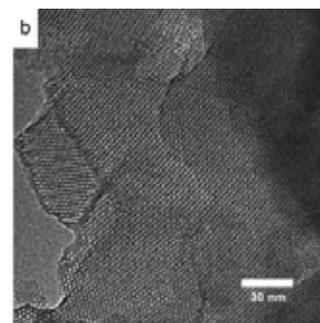
tronic transport. In this collaboration between the groups of Achim Hartschuh and Thomas Bein, the researchers have developed a new method for

strongly enhancing both features through the introduction of a modulating agent in the synthesis. This modulator competes with one of the building blocks

during the solvothermal COF growth, resulting in highly crystalline frameworks with greatly increased domain sizes reaching several hundreds of nanometers. The resulting materials feature fully accessible pores with an internal surface area of over  $2000 \text{ m}^2\text{g}^{-1}$ . Visualization of an -SH functionalized modulating agent via iridium staining revealed that the COF domains are terminated by the modulator. Using functionalized modulators, this synthetic approach thus also provides a new and facile method for the external surface functionalization of COF domains, providing accessible sites

for post-synthetic modification reactions. The researchers demonstrate the feasibility of this concept by covalently attaching fluorescent dyes and hydrophilic polymers to the COF surface. They anticipate that the realization of highly crystalline COFs with the option of additional surface functionality will render the modulation concept beneficial for a range of applications including gas separations, catalysis, and optoelectronics.

■ **M. Calik, T. Sick, M. Dogru, M. Doeblinger, S. Datz, H. Budde, A. Hartschuh, F. Auras, and T. Bein:** *From Highly Crystalline to Outer Sur-*



**Figure 1:** TEM micrographs of COF-5 (made from hexahydroxytriphenylene and benzene-1,4-diboric acid) crystalline domains with 10 mol% modulator added. The mono-functional modulator was 4-mercaptophenylboronic acid.

*face-Functionalized Covalent Organic Frameworks- A Modulation Approach;* *J. Am. Chem. Soc.* 138 (4), 1234-1239 (2016)

4

## NONEQUILIBRIUM AT THE MICROSCALE: FROM BIOTECHNOLOGY FOR MEDICINE TO UNRAVELING THE EMERGENCE OF LIFE

**Prof. Dieter Braun (LMU München, Physics Department)**

■ [www.biosystems.physik.lmu.de](http://www.biosystems.physik.lmu.de)

The Braun lab could detect with microscale thermophoresis in the blood plasma of patients the affinity of protease inhibitors. The finding demonstrates an assay capable of deciphering functional deviations from *in vitro* inhibition data by combining concentration and affinity measurements. The finding shows how nanoscience results can lead to applications in medical studies. They could find that the elastase is strongly modulated by so-far overlooked additional binding partners from the plasma. In addition, a study of amyloid fibrils, playing a large

role in neurodegenerative disorders, microscale thermophoresis could determine states of fiber growth and measure binding of ligands as possible therapeutic targets. The Braun lab continues their effort in deciphering the emergence of life on Earth. In a publication of Christof Mast in *Angewandte*, he could show how a temperature gradient induces the formation of micrometer-sized gels. In a way, these structures, larger and more random than DNA origami, create a phase transition of DNA with a macroscale phenotype for

selection and very high concentrations for RNA-world-type catalytic reactions. Most notably, Christof Mast showed how already single base pair mismatches in the phase transition decides on whether the gel is formed or not. The finding enables interesting possibilities on chirality selection and replication based on phase transitions. In a theoretical study, the Braun lab has revealed that already very flat thermal gradients - on the order of 100K over one meter - is capable to strongly accumulate and thermally cycle DNA for replication. This is a

2000-fold flatter gradient than shown before and enables molecular evolution to happen in a much larger range of boundary conditions in volcanic rock. New biotechnologies at the boundary to biology were also developed. Local photochemical reactions allow to create pH and electrical potential gradients, leading to local electrophoresis. Similar to thermophoresis, but now without convection artifacts, binding of aptamers to proteins could be measured. In addition, a new way to detect the diffusion of single fluorescence molecules in developing *Drosophila* could be shown with a novel reflected light sheet microscopy technique. The shown new microscopy will be helpful in studying single molecules or complexes in multicellular organisms.

■ **T. Dau, E. Edeleva, S. Seidel, R. Stockley, D. Braun, and D. Jenne:** *Quantitative analysis of protease recognition by inhibitors in plasma using microscale thermophoresis*; Scientific Reports, doi: 10.1038/srep35413 (2016)

**M. Wolff, J. Mittag, T. Herling, E. De Genst, C. Dobson, T. Knowles, D. Braun, and A. Buell:** *Quantitative thermophoretic study of disease-related protein aggregates*; Scientific Reports, doi:10.1038/srep22829 (2016)

**F. Greiss, M. Deligiannaki, C. Jung, U. Gaul, and D. Braun:** *Single molecule imaging in living Drosophila embryos with reflected light-sheet microscopy*; Biophysical Journal, doi: 10.1016/j.bpj.2015.12.035 (2016)

**L. Keil, M. Hartmann, S. Lanzmich, and D. Braun:** *Probing of molecular replication and accumulation in shallow heat gradients through numerical simulations*; PCCP, doi: 10.1039/C6CP00577B (2016)

**F. M. Möller, M. Kieß, and D. Braun:** *Photochemical microscale electrophoresis allows fast quantification of biomolecule binding*; JACS, doi: 10.1021/jacs.6b01756 (2016)

**M. Morasch, D. Braun, and C. B. Mast:** *Heat-Flow-Driven Oligonucleotide Gelation Separates Single-Base Differences*; Angewandte Chemie, doi: 10.1002/anie.201603779 (2016)

## 5

### A FORCE-SENSING PROTEIN IN THE BLOOD FLOW\*

**Dr. Martin Benoit (LMU München, Physics Department) ■ [www.biophysik.physik.lmu.de](http://www.biophysik.physik.lmu.de)**

**Prof. Jan Lipfert (LMU München, Physics Department) ■ [www.molecularbiophysics.physik.lmu.de](http://www.molecularbiophysics.physik.lmu.de)**

Von Willebrand factor (VWF) is a multimeric plasma glycoprotein that is essential for blood clotting (hemostasis), and dysfunction of VWF causes severe bleeding disorders. Under normal blood flow conditions, VWF circulates in the bloodstream in a globular, inactive conformation, but at sites of vascular injury becomes activated upon abrupt elongation by increased hydrodynamic forces. VWF strongly binds to the

injured vessel wall as well as to platelets, thus facilitating formation of a hemostatic platelet plug at the site of vascular injury and initiating thrombus formation. By atomic force microscopy (AFM)-based single-molecule force spectroscopy (SMFS) and AFM imaging experiments, the structure and mechanics of VWF dimers were assessed. In particular SMFS uncovered a strong and specific interaction within VWF dimers at forces above

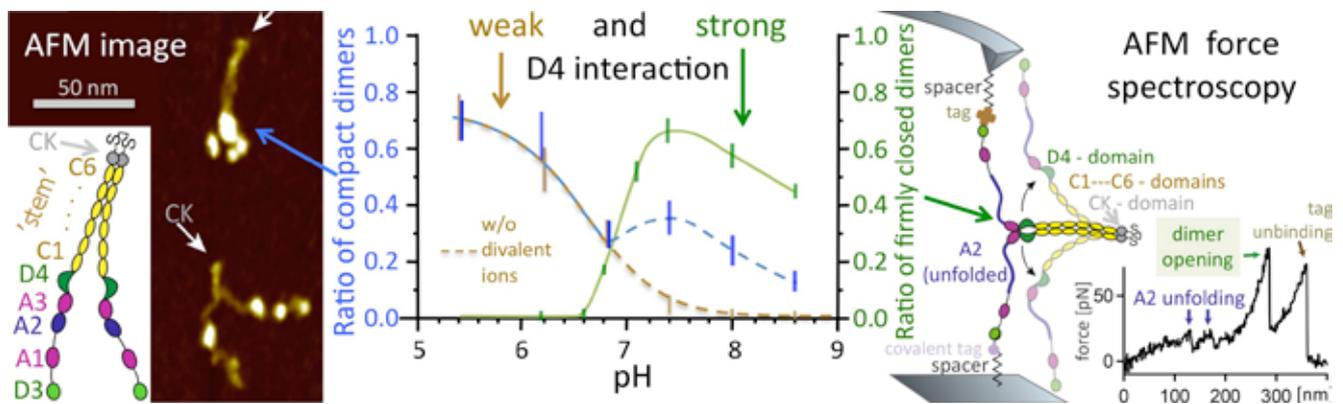
approximately 50pN<sup>(1)</sup>. This interaction involving the VWF D4 domain corresponds to a firmly closed conformation of the VWF dimers at pH values above 7, i.e. in the physiologically relevant pH range (green trace in Fig.1). Determining the fraction of compact VWF dimers in AFM images suggested further pH-dependent weak interactions (brown trace in Fig.1) within the VWF dimers at forces far below the force resolu-

tion of the AFM (~10pN). These weak interactions involve as well the VWF-D4 domain, but also the six C domains in VWF's so-called "stem" region. Importantly, the discovered interactions fine-tune the sensitivity of VWF to hydrodynamic forces in a pH-dependent manner<sup>(1,2)</sup>. These unexpected findings about VWF mechanics are not only intriguing from a single-molecule biophysics point of view, but also have far-reaching medical implications with respect to blood clotting and bleeding

disorders which will be further addressed within the collaborative research network SHENC (DFG FOR 1543).

■ **J. P. Müller, A. Löff, S. Mielke, T. Obser, L. K. Bruetzel, W. Vanderlinden, J. Lipfert, R. Schneppenheim, and M. Benoit:** *pH-Dependent Interactions in Dimers Govern the Mechanics and Structure of von Willebrand Factor*; *Biophysical Journal*, doi:10.1016/j.bpj.2016.06.022 (2016)

**J. P. Müller, S. Mielke, A. Löff, T. Obser, C. Beer, L. K. Bruetzel, D.A. Pippig, W. Vanderlinden, J. Lipfert, R. Schneppenheim, M. Benoit:** *Force sensing by the vascular protein von Willebrand factor is tuned by a strong intermonomer interaction*; *PNAS*, doi: 10.1073/pnas.1516214113 (2016)



**Figure 1:** AFM image of a compact (blue arrow) and a non-compact VWF dimer (white arrows indicate the dimerization site at the CK domain; further details on VWF domains in the schematic inset). The ratio of compact dimers decreases with increasing pH in the absence of divalent ions (dashed brown trace). In the presence of divalent ions however, which are crucial for formation of a strong intradimer interaction, a maximum appears at pH 7.4 (dashed blue trace). By state of the art AFM force spectroscopy, the ratio of force traces showing the characteristic force peak of the strong intradimer opening (very right small green arrow) was quantified as a function of pH (ratio of firmly closed dimers; green trace). Thus, it could be concluded that compactness of VWF dimers under acidic conditions is promoted by weak interactions, whereas it is promoted by a strong interaction at pH values around the physiological value of 7.4. Both the weak and the strong interactions crucially involve VWF's D4 domain, as inferred from measurements on a dimeric VWF construct lacking the D4 domain.

## TOXICITY OF NANOPARTICLES EMITTED BY CATALYTIC CONVERTERS OF AUTOMOBILES/ENVIRONMENTAL POLLUTION

Prof. Christoph Bräuchle (LMU München, Chemistry Department)

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Dr. Hanna Engelke (LMU München, Chemistry Department)

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Prof. Achim Wixforth (Universität Augsburg, Institut für Physik)

■ [www.physik.uni-augsburg.de/exp1/mitarbeiter/wixforth\\_achim/](http://www.physik.uni-augsburg.de/exp1/mitarbeiter/wixforth_achim/)

Investigation of the interaction between endothelial cells and nanoparticles emitted by catalytic converters of automobiles.

Although catalyst-derived particles are recognized as growing burden added to environmental pollution, very little is known about their health impact. Platinum-decorated ceria nanoparticles are used as model compounds for the actual emitted particles and focus on their fast uptake and association with mitochondria, the cell's powerhouse. Using live-cell imaging and electron microscopy it is demonstrated, that 46 nm platinum-decorated ceria nanoparticles can rapidly penetrate cell membranes and reach the cytosol. Moreover, if suitably targeted, these particles are able to selectively attach to mitochon-

dria. These results are complemented by cytotoxicity assays, thus providing insights into the biological effects of these particles on cells. Interestingly, no permanent membrane disruption or any other significant adverse effects on cells were observed. The unusual uptake behavior observed for 46 nm nanoparticles was not observed for equivalent but larger 143 nm and 285 nm platinum-decorated particles. The results demonstrate a remarkable particle size effect in which particles smaller than ~50–100 nm escape the usual endocytic pathway and translocate directly into the cytosol, while particles larger than ~150 nm are internalized by conventional endocytosis. Since the small particles are able to bypass endocytosis, they could

be explored as drug and gene delivery vehicles. Platinum-decorated nanoparticles are therefore highly interesting in the fields of nanotoxicology and nanomedicine.

■ **A.A. Torrano, R. Herrmann, C. Strobel, M. Rennhak, H. Engelke, A. Reller, I. Hilger, A. Wixforth, C. Bräuchle:** *Cell Membrane Penetration and Mitochondrial Targeting by Platinum-Decorated Ceria Nanoparticles*; *Nanoscale* 8, 13352 (2016)

## FORMATION OF VORTEX PATTERNS OF ACTIVE CURVED POLYMERS ON MEMBRANES\*

Prof. Erwin Frey (LMU München, Physics Department)

■ [www.theorie.physik.uni-muenchen.de/lsfrey](http://www.theorie.physik.uni-muenchen.de/lsfrey)

A critical component of the bacterial cell division machinery is a contractile polymer structure, called Z-ring, which performs cytokinesis. Rather than being a single, closed polymer ring, the Z-ring is composed of multiple, overlapping FtsZ filaments. However, how self-organization into this structure occurs, remains unknown and is subject to extensive research. Recent experiments [Loose and Mitchison (2013), Nat. Cell. Biol. 16, 38] of FtsZ on a supported lipid membrane have shown that FtsZ polymerizes into curved polymer filaments, which effectively move via treadmilling. These filaments collect into dynamic rings, which resemble the Z-ring in size and structure. The effect of chirality and directed motion on the collective dynamics remains, however, poorly understood. In this project, the question how these systems self-organize into



Figure 1: Image Christoph Hohmann, NIM

different patterns was approached by using concepts from the theory of active matter. In the work of J. Denk, L. Huber, E. Reithmann, and E. Frey active FtsZ polymers were modeled by studying self-propelled particles that move along circular, chiral paths. For intermediate polymer densities, the study predicts self-organization into vortex structures, which recall the ring patterns observed by Loose and Mitchison. The results have been consolidated by the phenomenological agreement of two different approaches: Brownian dynamics simulations and a kinetic Boltzmann approach were employed to study these systems on microscopic and mesoscopic length scales, respectively. Thereby the team of Prof. Frey obtained a phase diagram featuring a confined parameter region of steady, dense swirls. In the Boltzmann framework, they determined the nature and stability of patterns and quantify all corresponding phase transitions. Notably, the onset of pattern formation is described by an extended complex Ginz-

burg-Landau equation that represents an interesting mathematical problem in its own right. Applying their theory to treadmilling FtsZ polymers - the main motivation of the project - shows that steric interactions already suffice to obtain a vortex phase. The generic and robust existence of such a vortex phase is important, as it might facilitate Z-ring formation.

In a broader perspective, the study extends previous work on systems of self-propelled particles where soliton waves accompany the onset of collective motion. The authors find that curved motion inhibits these wave patterns in favor of vortices. Interestingly, the phase analysis is independent of curvature and therefore also valid for straight-moving particles.

■ **J. Denk, L. Huber, E. Reithmann, E. Frey:** *Active Curved Polymers form Vortex Patterns on Membranes*; Phys. Rev. Lett 116 (17),178301 (2016)

## DESIGNER CELLULOSOMES

Prof. Hermann E. Gaub (LMU München, Physics Department)

■ [www.biophysik.physik.lmu.de](http://www.biophysik.physik.lmu.de)

Prof. Michael A. Nash (University of Basel, Department of Chemistry and ETH Zurich, Department of Biosystems Science and Engineering)

■ [www.chemie.unibas.ch/~nashm](http://www.chemie.unibas.ch/~nashm)

Protein receptor-ligand pairs are widely probed by single molecule force measurements. In particular stronger receptor-ligand pairs as they are found in cellulosomes are increasingly used as specific molecular „handles“ in single-molecule experiments respectively (Fig.1A). By genetic engineering and enzymatic ligations such handles are fabricated to the molecule of interest together with known marker domains (also referred to as „finger-prints“), providing unique unfolding signatures to identify

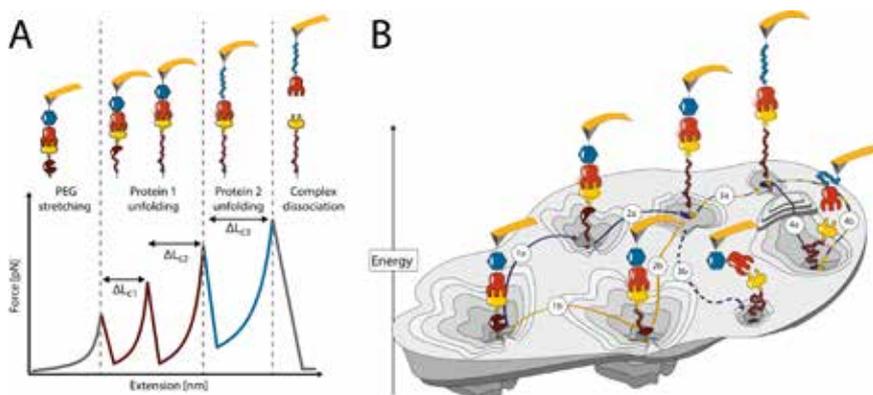
specific single-molecule interactions in a force-distance trace (Fig.1A).

Equipped with such sophisticated polyprotein and receptor-ligand complexes forces to open receptor-ligand pairs as well as forces to unfold proteins were measured and evaluated with high precision. Interestingly the influence of the binding strength of molecular handles to the unbinding kinetics of the probed interactions could be quantified and now allows for predicting the unbiased kinetics. Hereby detailed (sub-)pathways (Fig.1B)

of the unfolding, and unbinding forces of a polyproteinic receptor-ligand complex became quantitatively evident.

The so far weakest member of the cohesin-dockerin binding partner family was found to be the toxin anchor from the pathogen *Clostridium perfringens*. Of course many more molecular interactions were and will be addressed with this powerful molecular toolbox.

With all the components thoroughly characterized, designer cellulosomes are assembled either by single molecule cut & paste or by self assembly of functional units.



**Figure 1:** **A)** „Fingerprints“ (brown and blue) are site-specifically and covalently attached to the cantilever and surface. Receptor (orange) and ligand (yellow) form a stable cohesin-dockerin receptor-ligand complex. Fingerprints can be individual sub-domains, or repetitive polyproteins in their own right. A typical force-extension trace is shown below with unfolding of the fingerprints, followed by rupture of the receptor ligand complex. In order to observe unfolding of the fingerprints in sufficient numbers, their most probable unfolding force should lie well below the most probable rupture force of the complex for the given loading rate. **B)** graphical reconstruction of the multidimensional unfolding and unbinding pathways of such a complex.

■ **L. F. Milles, E. A. Bayer, M. A. Nash, H. E. Gaub: Mechanical Stability of a High-Affinity Toxin Anchor from the Pathogen *Clostridium perfringens*; Journal of Physical Chemistry B - Klaus Schulten Memorial Issue, 10.1021/acs.jpccb.6b09593 (2016)**

W. Ott, T. Nicolaus, H. E. Gaub, and M. A. Nash: *Sequence-Independent Cloning and Post-Translational Modification of Repetitive Protein Polymers through Sortase and Sfp-Mediated Enzymatic Ligation*; *Biomacromolecules*, doi:10.1021/acs.biomac.5b01726 (2016)

W. Ott, M. A. Jobst, C. Schoeler, H. E. Gaub, M. A. Nash: *Single-molecule force spectroscopy on polyproteins and receptor-ligand complexes: The current toolbox*; *Journal of Structural Biology*; doi:10.1016/j.jsb.2016.02.011 (2016)

C. Schoeler, T. Verdorfer, H. E. Gaub, and M. A. Nash: *Biasing effects of receptor-ligand complexes on protein-unfolding statistics*; *Physical Review*, DOI:10.1103/PhysRevE.94.042412 (2016)

9

## STUDYING AND OPTIMIZING CHARGE TRANSPORT IN HYBRID HALID PEROVSKITE SOLAR CELL MATERIALS

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■ [www.cup.uni-muenchen.de/pc/hartschuh](http://www.cup.uni-muenchen.de/pc/hartschuh)

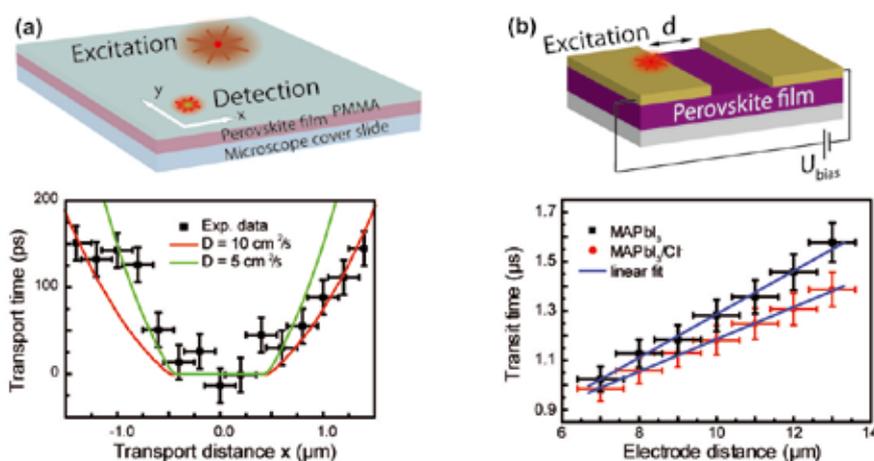
Prof. Thomas Bein (LMU München, Chemistry Department)

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High power conversion efficiencies, facile solution processing and compatibility with current printing technology render metal halide perovskites a new class of materials for large-scale photovoltaic systems. Key for an efficient extraction of photo-generated carriers is the combination of low non-radiative relax-

ation rates leading to long carrier lifetimes and rapid diffusive transport. The latter, however, is difficult to assess directly with reported values varying widely for metal halide perovskites materials. We used a contact-less approach for the visualization of the charge carrier diffusion length in thin films based on

time-resolved confocal detection of photoluminescence (PL) at varying distances from the excitation position (Figure 1(a)). Our measurements on chloride-treated methylammonium lead iodide (MAPI) thin films, the material for which high solar cell efficiencies of up to 19% have been reported, reveal a charge carrier diffusion length of 5.5 - 7.7  $\mu\text{m}$  and diffusion constants around  $5 \text{ cm}^2 \text{ s}^{-1}$ , similar to GaAs thin films. We complement these PL studies with electrical transport measurements using the time-of-flight technique. Laterally contacted MAPI thin films (Figure 1(b)) are found to exhibit charge carrier mobilities on the order of 2-3  $\text{cm}^2/\text{Vs}$ . These values are substantially lower than those calculated from the optically determined diffusion constants using the Einstein relation. This could be assigned to the different probing regimes



**Figure 1:** Time-resolved investigations of charge carrier transport in metal halide perovskite thin films using (a) focused laser excitation and remote detection of photoluminescence and (b) transient photocurrent detection.

of the employed techniques: While the optical measurement focuses on local transport, the electrical measurement analyzes charge transport over many microns along multiple grain boundaries. We further find that the optoelectronic properties of MAPI films can be improved by adding a chloride containing salt to the precursor solution during film synthesis. *In-situ* photoluminescence lifetime measurements indicate that the addition of chloride results in slower crystals growth and a smaller density of defects. Our results contribute to our understanding of photo-initiated processes in perovskite

materials and their correlation with material morphology and composition and could help to further improve the performance of perovskite-based solar cells.

- **I. Grill, K. Handloser, F. C. Hanusch, N. Giesbrecht, T. Bein, P. Docampo, M. Handloser, A. Hartschuh:** *Controlling crystal growth by chloride-assisted synthesis: Towards optimized charge transport in hybrid halide perovskites*; *Solar Energy Materials and Solar Cells*, DOI: 10.1016/j.solmat.2016.11.021 (2016)
- **K. Handloser, N. Giesbrecht, T. Bein, P. Docampo, M. Handlos-**

**er, A. Hartschuh:** *Contact-less Visualization of Fast Charge Carrier Diffusion in Hybrid Halide Perovskite Thin Films*; *ACS Photonics*, DOI: 10.1021/acsp Photonics.5b00562 (2016)

**A. Binek, I. Grill, N. Huber, K. Peters, A. G. Hufnagel, M. Handloser, P. Docampo, A. Hartschuh, Thomas Bein:** *Control of Perovskite Crystal Growth by Methylammonium Lead Chloride Templating*; *Chem. Asian J.*, DOI: 10.1002/asia.201501379 (2016)

10

## EXCITON LOCALIZATION IN CARBON NANOTUBES

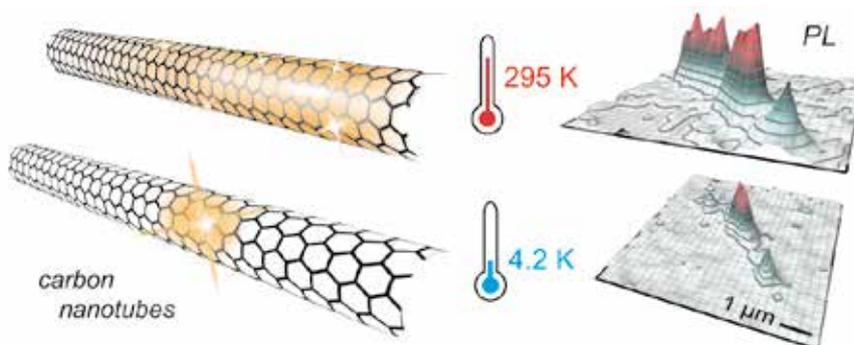
**Prof. Alexander Högele (LMU München, Physics Department)**

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A light source that emits only one photon at a time is an invaluable tool for quantum communication and cryptography. Quasi-zero-dimensional systems such as atoms, nitrogen vacancies in diamond, or quantum dots emit photons one by one when excited by laser light. For one-dimensional carbon nanotubes with spatially extended photoluminescence from diffusive excitons at room-temperature, however, such highly non-classical emission of single photons at cryogenic temperatures is surprising. The group headed by Alexander Högele has now uncovered temperature-driven exciton localization at environmental disorder as a

generic feature of carbon nanotubes. Irrespective of the fabrication method, carbon nanotubes tend to localize excitons in quasi-zero-dimensional traps with potential depths that

exceed the thermal energy at cryogenic temperatures. By virtue of exciton localization, a carbon nanotube fractionalizes into a collection of independent and spatially separated quantum



**Figure 1:** Spectroscopy of individual carbon nanotubes reveals the cross-over from the diffusive to the localized regime of nanotube excitons at cryogenic temperatures as a ubiquitous phenomenon in micelle-encapsulated and as-grown single-walled carbon nanotubes.

emitters with low two-photon emission probability. As such, nanotubes qualify as potentially viable sources of quantum light with emission wavelength that

can be matched to the telecom band by an appropriate choice of the nanotube diameter.

- **M. S. Hofmann, J. Noé, A. Kneer, J. J. Crochet, and A. Högele:** *Ubiquity of exciton localization in cryogenic carbon nanotubes*; *Nano Lett.* 16, 2958 (2016)

11

## PLASMON-EXCITON COUPLING USING DNA TEMPLATES\*

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**Prof. Tim Liedl (LMU München, Physics Department)**

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Strong-coupled systems, which exhibit coherent energy exchange, manifests itself in the emergence of new hybrid eigenstates which can be studied with optical spectroscopy. Strongly coupled systems are of high interest to study fundamental quantum phenomena, such as Fano resonance, Rabi splitting, and superradiance. One prospect to realize such systems is through interaction between metal plasmons and excitons. In our paper entitled "Plasmon-Exciton Coupling Using DNA Templates," we present a method to design and fabricate plasmon-exciton substrates self-assembled using DNA origami templates. The pre-programmable bottom-up approach of the DNA origami technique allows to position colloidal metal nanoparticles in configurations that have

custom-tuned plasmon resonances. For that, we designed the plasmon resonance of two nanoparticles with fixed interparticle gap distance (5 nm) to be in perfect overlap with the resonance of a J-aggregate exciton. With this approach, we studied the plasmon-exciton interactions of the hybrid nanostructure as a function of the detuning parameter, the nanoparticle radius. Our in-solution plexciton systems are programmed to self-assemble in solution, and take advantage of the field confinement from bringing colloidal nanocrystals in close proximity. The proposed technique provides unprecedented control in the design of plexcitonic systems, bringing this technology one step closer to practical applications as compared to all previously

proposed plexcitonic designs. Our work shows that rigid DNA template structures can serve as versatile building blocks for plasmonics as well as functional templates to study fundamental plasmon-exciton interactions. This paper is the first time DNA-Origami has been used to promote plasmon-exciton coupling. The potential applications of plexcitonic systems are manifold, and span multiple disciplines and range of applications such as new optical devices, light harvesting, to quantum information processing.

- **E.-M. Roller, C. Argyropoulos, A. Högele, T. Liedl, and M. Pilo-Pais:** *Plasmon-exciton coupling using DNA templates*; *Nano Lett.* 16, 5962 (2016)

## ULTRAFAST OPTICAL CONTROL OF GRAPHENE PLASMONS

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■ [www.softmatter.physik.uni-muenchen.de/personen/guests/fritz-keilmann1](http://www.softmatter.physik.uni-muenchen.de/personen/guests/fritz-keilmann1)

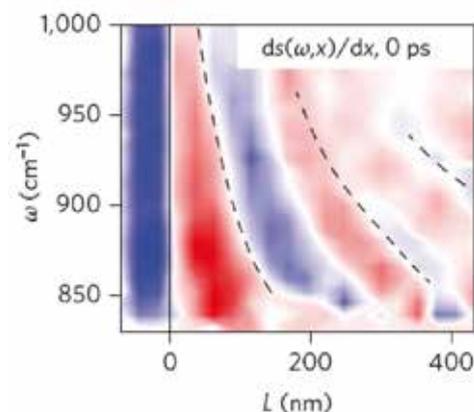
Monolayer graphene at low doping is not conductive enough to support mid-infrared plasmon polaritons. We show that sufficient conductivity is achievable transiently by optical pumping with a 100-fs near-infrared pulse. Furthermore, we probe both the phase velocity and the range of plasmon polaritons by plasmon interferometry, a method that has been pioneered by us before and that comprises steps (i) of launching plasmon polaritons from the metal tip of a scattering-type optical near-field microscope (commercialized by CeNS startup Neaspec GmbH), (ii) partially reflecting them from a closeby edge of the graphene crystal, and (iii) detecting them by registering the back-scattering efficiency of the tip as a function of distance  $L$  between tip and edge.

The figure shows a snapshot at the time of optical pumping, in the fashion of a spectroscopic line scan extending up to  $L = 430$  nm from the graphene edge, for a 15% wide mid-infrared spectrum where graphene plasmons exhibit strong dispersion. As example, the fringe spacing (separation of dashed curves) of 165 nm at  $900\text{ cm}^{-1}$  can be interpreted as half a plasmon wavelength of 330 nm whence that plasmon propagates as slowly as 3% only of the free-space light velocity.

Delaying the spectral probing from the pump pulse allows to follow in detail the ultrafast changes of plasmon dispersion and thus of the complex conductivity which is mainly governed by the density, scattering rate, and temperature of the excited free charge carriers, until their full disappearance after a few ps.

Understanding the dynamics of nonequilibrium plasmons is expected to reveal damping effects of acoustic phonon scattering and also of electron-electron scattering due to non-intentional, possibly nano-scale doping, and is prerequisite for the aim of applying high-mobility graphene for manipulating light at ultrasmall length and time scales.

■ **G.X. Ni, L. Wang, M.D. Goldflam, M. Wagner, Z. Fei, A.S. McLeod, M.K. Liu, F. Keilmann, B. Özyilmaz, A.H. Castro Neto, J. Hone, M.M. Fogler, and D.N. Basov:** *Ultrafast optical switching of infrared plasmon polaritons in high-mobility graphene*; *Nature Materials*, DOI:10.1038/NPHOTON.2016.45 (2016)



**Figure 1:** Transient plasmon interference fringes, standing electric fields at the  $L = 0$  edge of monolayer graphene, acquired for a continuum of mid-infrared frequencies ( $1000\text{ cm}^{-1}$  corresponds to  $10\text{ }\mu\text{m}$  wavelength) at the time of optical pumping.

## COORDINATIVE SELF-ASSEMBLY OF HIS-TAGGED UNITS WITH METAL-ORGANIC FRAMEWORKS

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Prof. Thomas Bein (LMU München, Department of Chemistry)

■ [www.bein.cup.uni-muenchen.de](http://www.bein.cup.uni-muenchen.de)

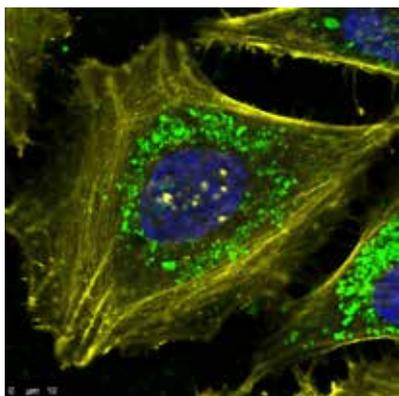
Dr. Stefan Wuttke (LMU München, Department of Chemistry)

■ [www.wuttkegroup.de](http://www.wuttkegroup.de)

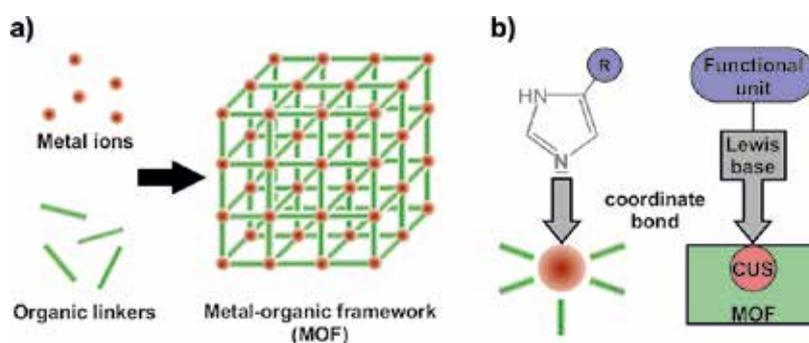
Prof. Joachim Rädler (LMU München, Department of Physics)

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Self-assembly of individual units into multicomponent complexes is a powerful approach for the generation of functional super-structures. The junior research groups of Ulrich Lächelt and Stefan Wuttke as well as the established groups of Ernst Wagner, Thomas Bein and Joachim Rädler used their interdisciplinary expertise in materials science, nanotechnology, physics and biotechnology to develop a novel concept for the assembly of different oligo-



**Figure 2:** Confocal laser scanning microscopy image of a HeLa cell treated with Zr-fumarate MOF NPs functionalized with His-tag containing recombinant green fluorescent protein (GFP). Green, GFP fluorescence; yellow, actin staining with rhodamine-phalloidin; blue, nuclear staining with DAPI.



**Figure 1:** Illustration of coordinative self-assembly of His-tagged molecules with MOF NPs: **a)** molecular composition of MOFs; **b)** coordinative bond between the imidazole group of histidines acting as Lewis base and coordinatively unsaturated metal sites (CUS) acting as Lewis acid.

histidine (His-tag) containing functional units, peptides and proteins, on the outer surface of metal-organic framework nanoparticles (MOF NPs).

The concept uses the interaction between the imidazole function of histidine acting as Lewis base and coordinatively unsaturated metal sites (CUS) present on the external surface of MOF NPs (Fig. 1). The coordinative interaction of functionalized His-tags with MOF NPs provides His-tag length and MOF species dependent binding as well as rapid release upon acidification. Evidence for simultaneous assembly of different functional units with MOF NPs and their successful transport into living

cells (Fig. 2) illustrate the promising potential of the self-assembly approach for the generation of multifunctional NPs and future biological applications.

The MOF structural designability at the molecular level (so far 20.000 different MOF structures are known) together with the high number of accessible His-tagged functional units opens the perspective to generate a variety of “self-assembling multifunctional coordination particles” (SAMCOPs) by simple combinatorial and stoichiometric mixing. In this respect, the work presents a versatile functionalization concept of MOF NPs with great potential for co-delivery of

proteins, drugs or other pharmacologically active agents, including those that can be adsorbed within the pore systems.

■ R. Röder, T. Preiß, P. Hirschle, B. Steinborn, A. Zimpel, M. Höhn, J. Rädler, T. Bein, E. Wagner, S. Wuttke, U. Lächelt: *Multifunctional*

*Nanoparticles by Coordinative Self-Assembly of His-Tagged Units with Metal–Organic Frameworks*; *J. Am. Chem. Soc.* 139 (6), 2359–2368 (2017)

14

## ON-SURFACE SYNTHESIS OF HIGHLY STABLE MOLECULAR SIERPINSKI TRIANGLES

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

■ [www.2d-materials.com](http://www.2d-materials.com)

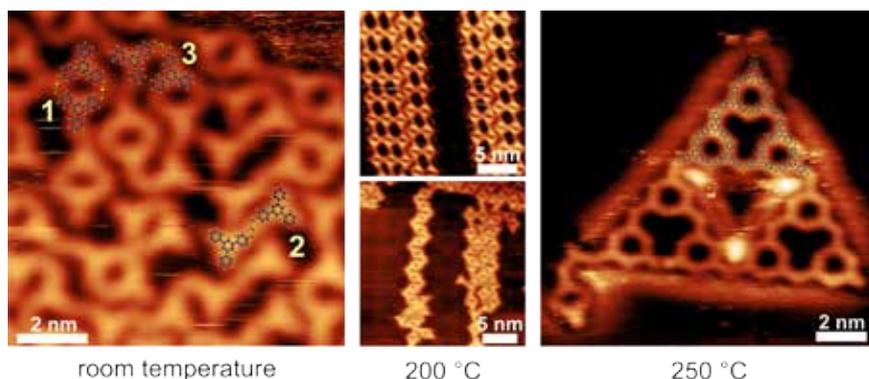
Molecular materializations of Sierpinski triangles were achieved by on-surface synthesis on Au(111) from 1,3,5-tris(4-mercaptophenyl)benzene (TMB) – a threefold symmetric thiol functionalized aromatic molecule. Owing to their fractal dimensionality these molecular nanostructures are anticipated to possess exotic optical, electronic, and magnetic properties. Interestingly, theoretical predictions triggered experimental work on the self-assembly of Sierpinski triangles from simple molecular building blocks. While the recently demonstrated examples are stabilized by relatively weak interactions as halogen, hydro-

gen or metal-coordination bonds, applications would greatly benefit from more stable molecular architectures. Hence, the aim of the project was the realization of molecular Sierpinski triangles that are stabilized by covalent intermolecular bonds. The applied synthetic strategy was to utilize thermally activated intermolecular coupling reactions on surfaces.

Initial room temperature deposition of TMB yielded seemingly disordered structures that were all based on only three distinct metal-organic binding motifs. Mild sample annealing at 200 °C increased the overall order by inducing a structural conversion

into extended metal-organic chains that were still based on the same binding motifs. Only annealing at higher temperatures afforded the desired molecular Sierpinski triangles. Accompanying Monte Carlo simulations showed that the combination of threefold symmetric building blocks with 120° angles for newly formed intermolecular bonds accounts for formation of these regular fractals. This favorable bond geometry was realized by a conversion of the metal-organic

**Figure 1:** Scanning Tunneling Microscopy images of TMB on Au(111) acquired after different thermal treatments. After room temperature deposition less well ordered structures emerged that feature only three distinct metal-organic binding motifs (cf. overlays). Heating to 200 °C results in metal-organic chains still based on the similar binding motifs, whereas covalent Sierpinski triangles with intermolecular thioether linkages were observed. After heating to 250 °C. The overlay with the respective DFT-optimized structure yields a perfect match.



thiolate-gold-thiolate linkages into covalent thioether bonds. Structural simulations on the density functional theory level feature a perfect match with the experimentally observed structures.

■ **A. Rastgoo-Lahrood, N. Martsinovich, M. Lischka, J. Eichhorn, P. Szabelski, D. Nieckarz, T. Strunskus, K. Das, M. Schmittel, W.M. Heckl, and M. Lackinger:** *From Au-Thiolate Chains to Thioether Sierpiński*

*Triangles: The Versatile Surface Chemistry of 1,3,5-Tris(4-Mercaptophenyl)Benzene on Au(111); ACS Nano 10(12), 10901-10911 (2016)*

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## DYNAMICS OF THE SPLICESOME

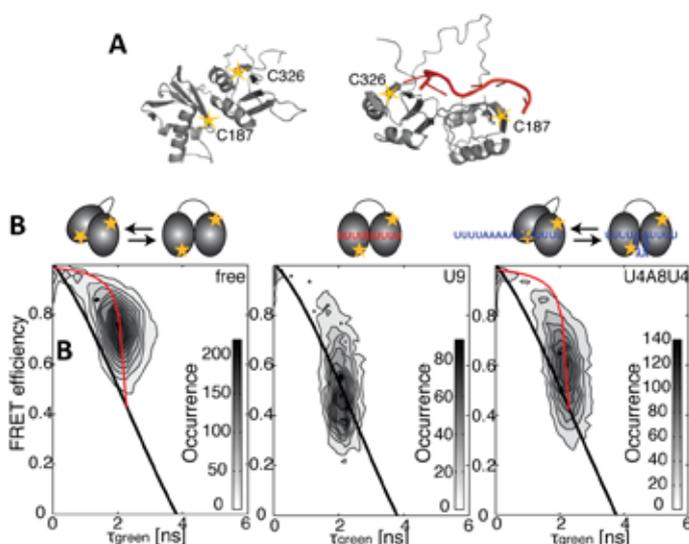
Prof. Don C. Lamb (LMU München, Department of Chemistry)

■ [www.cup.uni-muenchen.de/pc/lamb](http://www.cup.uni-muenchen.de/pc/lamb)

Removal of introns in messenger RNA is essential for maturation of the RNA and proper protein expression. The spliceosome controls and regulates the splicing process. Recognition of regulatory sequences on the

RNA sequence by splicing factors is an important early step in assembly of the spliceosome. To investigate the recognition of the 3' splice site in pre-messenger RNA introns by the splicing factor U2 auxiliary factor (U2AF),

we combined single molecule fluorescence experiments with NRM. From the single-pair Förster Resonance Energy Transfer (spFRET) experiments, we showed that the U2AF complex is dynamic, fluctuating on the submillisecond timescale between an open and closed configuration. Recognition of the polypyrimidine tract (Py-tract) involves a shift in the equilibrium population towards the open conformation. The amount of the shift correlates with the strength of the Py-tract. For weaker Py-tracts, the presence of the small subunit, U2AF35, aids in recognition of the splice site. This is performed by causing a shift in the population of the RNA binding domains of the



**Figure 1:** Conformation and dynamics of the spliceosome auxiliary factor U2AF65. **(A)** Two structures of U2AF65, determined from NMR, are shown. Left a closed structure (PDB 2YH0) is observed in the absence of RNA. Right, with RNA-bound, the structure takes on an open conformation (PDB 2YH1). The labeling sites used for spFRET experiments, C187 and C326, are shown as stars. **(B)** Histograms of donor lifetime versus spFRET efficiency are plotted in the absence of RNA (9,160 molecules), in the presence of 5  $\mu\text{M}$  U9-RNA (10,015 molecules), or in the presence of 20  $\mu\text{M}$  U4A8U4-RNA (12,083 molecules). Molecules with a static conformation during a burst will fall on the polynomial static FRET line (black), whereas molecules undergoing conformational dynamics will deviate from this line (dynamic FRET curve; red line). The spliceosome shows clear dynamics between an open and closed conformation in the absence of RNA or for a weak polypyrimidine tract. For the U9-RNA, the protein is locked in the open conformation. Schematics are shown above as a simple interpretation of the histograms. Copyright 2016 PNAS.

U2AF65 subunit towards the open conformation. This could explain why the presence of U2AF35 is required for the splicing of introns with a weak Py-tract as observed in eukaryotic systems. The picture that emerges from this investigation is that the efficiency of splicing correlates with stabilization of the open conformation of U2AF65. U2AF65 fluctuates between an open and closed conformation in

the absence of RNA and formation of the protein-RNA complex utilizes a conformational selection mechanism favoring the open conformation. While strong Py-tracts are readily recognized by U2AF65, the U2AF35 subunit is instrumental for stabilization of the open conformation in the presence of weak Py-tracts. Thus, the population shift to the open conformation is an essential step in assembly of the spliceosome.

■ **L. Voith von Voithenberg, C. Sánchez-Rico, H.-S. Kang, T. Madl, K. Zanier, A. Barth, L.R. Warner, M. Sattler, and D.C. Lamb: Recognition of the 3' splice site RNA by the U2AF heterodimer involves a dynamic population shift; PNAS 113, E7169 (2016)**

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## HYDROPHOBIC PROPERTIES OF BIOFILM-ENRICHED HYBRID MORTAR

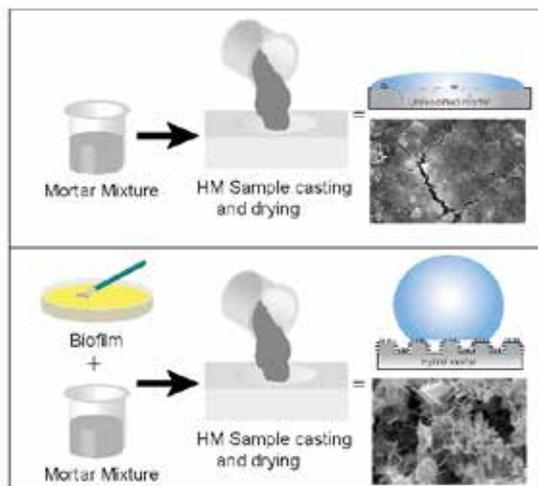
Prof. Oliver Lieleg (TU München, Institute of Medical Engineering)

■ [www.imetum.tum.de/forschung/biologische-hydrogele](http://www.imetum.tum.de/forschung/biologische-hydrogele)

Preventing water penetration by generating hydrophobic surfaces through coating or mixing approaches is a challenging task in many fields of material development. One field where water-resistant surfaces are critically needed is civil engineering: the durability of cement-based materials such as mortar and concrete typically suffers from water and chloride ingress, which corrodes load-bearing steel reinforcement elements integrated into the volume of the material. Most existing strategies to increase the water resistance of cementitious materials are based on an additional surface treatment of the material after the casting process or rely on integrating hydrophobic components into the bulk volume of the material. A complementary strategy could be a bulk modification of cemen-

titious materials by altering their mineralized nanostructures, such as ettringites. Controlling mineralization processes through bio-inspired approaches has already led to many new hybrid materials with astonishing properties. In this project, a mortar hybrid material was developed in which biomineralization processes were stimulated by adding a biological component, i.e., bacterial biofilm, to the inorganic mixture. Bacterial biofilms are ubiquitous communities of bacteria encased in a matrix of self-produced biopolymers. In such a biofilm matrix, the bacteria are able to resist various environ-

mental challenges, e.g., chemicals, desiccation, or removal



**Figure 1:** In the hybrid mortar material, biomineralization processes are stimulated by adding a biological component, i.e. bacterial biofilm, to standard mortar. The generated material exhibits increased roughness on the microscale and the nanoscale. Accordingly, the hybrid mortar not only resists wetting but also suppresses the uptake of water by capillary forces.

from surfaces. With this addition of biofilm to mortar, a material was generated that exhibits an increased roughness on the microscale and the nanoscale, and on both the outer and inner surface. Accordingly, the hybrid mortar not only resists wetting but also suppresses the uptake of water by capillary forces. Hydrophobic hybrid mortar cannot

only be obtained by using freshly harvested biofilms as an admixture, but also when the biological component is added as a lyophilized powder during the casting process. This may facilitate a later scale-up of the material production process and thus open avenues for applications in civil engineering.

■ **S. Grumbein, D. Minev, M. Tallawi, K. Boettcher, F. Prade, F. Pfeiffer, C.U. Große and O. Lileg:** *Hydrophobic Properties of Biofilm-Enriched Hybrid Mortar*; *Advanced Materials*, 37(5), 8138-8143 (2016)

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## SAXS DNA ORIGAMI

Prof. Jan Lipfert (LMU München, Physics Department)

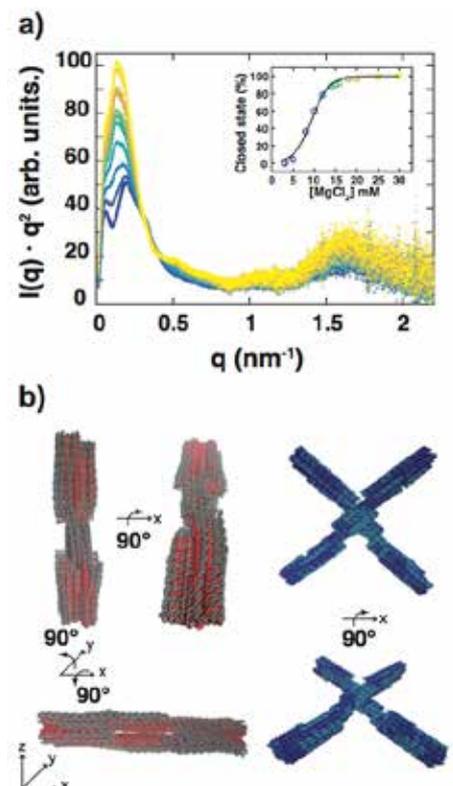
■ [www.biophysik.physik.uni-muenchen.de](http://www.biophysik.physik.uni-muenchen.de)

Prof. Hendrik Dietz (TU München, Physics Department)

■ [www.dietzlab.org](http://www.dietzlab.org)

DNA origami has emerged as an ideal tool to create biomimetic objects that can adopt specific conformations and carry out functions at the molecular scale ranging from nanometers to micrometers due to its chemical addressability and predictable base-pairing. Examples include both static structures in two- or three-dimensions and dynamic devices that can undergo controlled conformational changes. So far, structural characterization of DNA origami structures has predominantly relied on atomic force microscopy (AFM) imaging and negative-stain transmission electron microscopy (TEM), requiring immobilization of the samples on a surface and making it challenging to detect conformational changes upon variation in solution conditions. In our study, we demonstrates that small angle X-ray scattering (SAXS) can quantita-

tively determine the conformational changes of a DNA origami „switch“ device as a function of ionic strength in free solution. We performed solution SAXS measurements at the European Synchrotron Radiation Facility on a dynamic switch variant for varying  $\text{MgCl}_2$  concentrations (Figure 1a). The resulting scattering profiles could be described by a two-state fit, where the scattering data at each  $\text{MgCl}_2$  concentration is a linear superposition of the scattering, allowing for the determination of the populations at each salt concentration. The salt-dependence of the fraction closed



**Figure 1** (a) Scattering profiles (in Kratky representation) of the switch samples for  $\text{MgCl}_2$  concentrations from 3 mM (dark blue, bottom) to 30 mM (light yellow, top). Inset: fraction of closed switch particles determined from SAXS and fit of a two-state model (black line). (b) Structural models derived from the normal mode refinement. Initial models are in red and dark blue, refined model in grey and cyan.

could be fitted by a thermodynamic model that assumes a linear dependence of the free energy  $\Delta G$  on the ion concentration  $c$  (Fig.1b).

In addition, we compared our experimental data to scattering profiles from computer generated, idealized three-dimensional atomistic models, revealing systematic deviations between the experimental and theoretical profiles. We employed a normal

mode based elastic network model approach to refine the idealized atomistic models against the experimental SAXS data. The results of the refinement suggest that the DNA helices are deformed from the idealized geometries, consistent with electrostatic repulsion. Our results establish SAXS as a powerful tool to investigate conformational changes and solution structures of DNA

origami and we anticipate our methodology to be broadly applicable to increasingly complex DNA and RNA devices.

■ **L. K. Bruetzel, T. Gerling, S. M. Sedlak, P. U. Walker, W. Zheng, H. Dietz, and J. Lipfert:** *Conformational Changes and Flexibility of DNA Devices Observed by Small-Angle X-Ray Scattering; Nano Letters* 16:4871-9 (2016)

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## BENDING GOLD NANORODS WITH LIGHT\*

Dr. Theobald Lohmüller (LMU Munich, Physics Department)

■ [www.phog.physik.lmu.de/people/project-leaders/lohmuller\\_theobald](http://www.phog.physik.lmu.de/people/project-leaders/lohmuller_theobald)

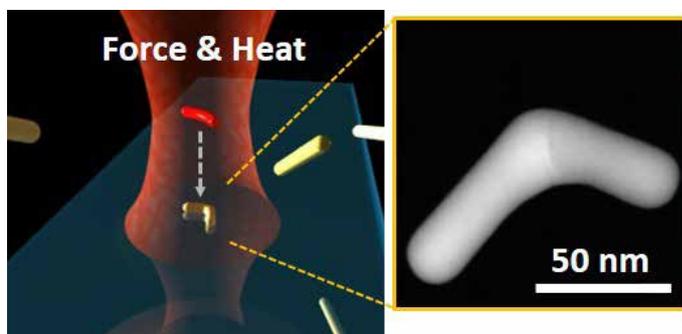
Plasmonic 'V-shaped' nanoantennas are important building blocks for the rational design of optical metamaterials and flat optical devices. The fabrication of V-shaped antenna arrays, however, is not a simple task. Electron beam lithography is widely used, but shows limitations when it comes to the fabrication of very small gold

nanostructures with high crystallinity and purity. The controlled assembly of gold nanoparticles from solution would be a preferred alternative, yet the chemical synthesis of V-shaped nanoparticles itself is already an outstanding challenge.

In this work, an elegant solution to this problem was developed.

For the first time it was shown that laser light can be applied to bend single gold nanorods in solution and, at the same time, to optically pattern the re-shaped particles with preferred orientation onto an underlying substrate. This new approach simultaneously leverages two modes of light-matter interactions, namely plasmonic heating and optical forces, to achieve a previously impossible feat for nanofabrication. Furthermore, a strategy was developed to precisely control the bending angle and to align the orientation of the bent rods on the substrate by tuning the laser conditions.

■ **A. Babynina, M. Fedoruk, P. Kühler, A. Meledin, M. Döblinger, T. Lohmüller:** *Bending Gold Nanorods with Light; Nano Letters* 16 (10), 6485-6490 (2016)



**Figure 1:** **Left:** Schematic illustration of the nanorod bending process. Gold nanorods in solution are simultaneously heated and pushed with a focused laser beam. **Right:** The bending angle of the nanorod is controlled by the laser power.

## DARK PHOTOCATALYSIS WITH 2D CARBON NITRIDES

Prof. Bettina V. Lotsch (LMU Munich, Department of Chemistry and MPI for Solid State Research, Stuttgart)

■ [www.cup.uni-muenchen.de/ac/lotsch](http://www.cup.uni-muenchen.de/ac/lotsch)

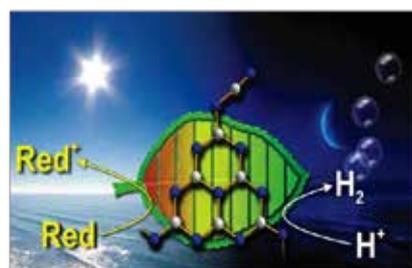
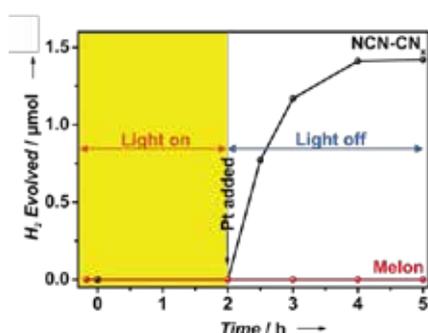
The rational development of carbon nitride photocatalysts for hydrogen evolution has been hampered by a lack of understanding of the structure – property – activity relationships in these semi-crystalline polymeric materials. We have therefore developed a rational approach to identify the catalytically relevant sites in heptazine-based carbon nitrides, which are often considered to be imperfections or crystal defects, and have then used this knowledge to synthesize highly active carbon nitride photocatalysts with external quantum efficiencies for hydrogen evolution exceeding 15%. Using molecular model photocatalysts, we have identified the cyanamide moiety as a possible “functional defect” innate to the prototypical carbon nitride photocatalyst Melon. Deliberate-

ly inserting this functional group into the carbon nitride backbone has led to a cyanamide-enriched 2D carbon nitride, notated as  $\text{NCN-CN}_x$ , which exhibits photocatalytic activity over 10 times higher than the archetype Melon under simulated sunlight. Upon photoreduction in the presence of a sacrificial electron donor,  $\text{NCN-CN}_x$  exhibits the unusual ability to “store” electrons as long-lived  $\pi$ -radicals, characterised by a colour change of the material from yellow to blue. We have exploited this effect for the time-delayed  $\text{H}_2$  evolution in a process illustrated in Fig. 1. After generation of the radical species by irradiation with light, the  $\text{H}_2$  evolution reaction is initiated by addition of a  $\text{H}_2$  evolution catalyst (Pt colloid) in the dark. The  $\text{H}_2$  evolution can

be triggered on demand even up to 12 h after irradiation. The temporal separation of the light and dark reactions of the water splitting process is akin to Photosystem I in natural photosynthesis, in which the photoexcited electrons are relayed across a complex electron transfer chain to prevent recombination and then utilized in the form of NADPH in the Calvin-Benson cycle for  $\text{CO}_2$  fixation in the dark. The ability of  $\text{NCN-CN}_x$  to decouple the light and dark reactions in one single, artificial material can be exploited for the production of storable solar fuels independent of the intermittency of solar irradiation.

■ V. W.-h. Lau, I. Moudrakovski, T. Botari, S. Weinberger, M. B. Mesch, V. Duppel, J. Senker, V. Blum, B. V. Lotsch: *Rational design of carbon nitride photocatalysts: Identification of cyanamide defects as catalytically relevant sites*; Nat. Commun. 7, 12165 (2016)

V. W.-h. Lau, D. Klose, H. Kasap, F. Podjaski, M.-C. Pigne, E. Reisner, G. Jeschke, B. V. Lotsch: *Dark photocatalysis: Storage of solar energy in carbon nitride for the time-delayed production of solar fuels*; Angew. Chem. Int. Ed. 56, 510 (2017)



**Figure 1:** Left: Illustration of the delayed photocatalytic hydrogen evolution process in the dark: No hydrogen is evolved during irradiation (yellow) without the presence of a hydrogen evolution catalyst, while hydrogen is evolved after the light is turned off and the catalyst (colloidal platinum) is added. Right: Schematic of the “dark photocatalysis”.

## PROTEIN CROWDING IN LIPID BILAYERS: NON-GAUSSIAN ANOMALOUS DIFFUSION

Prof. Ralf Metzler (University of Potsdam, Institute for Physics and Astronomy)

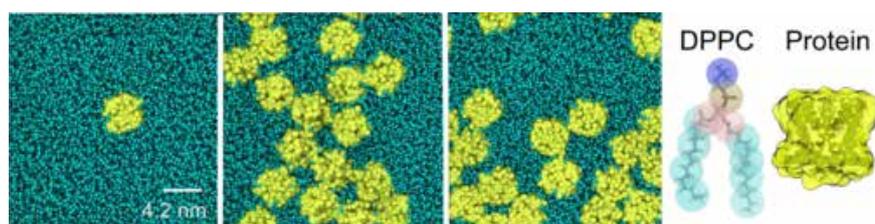
■ [www.agnld.uni-potsdam.de/~metz/index.html](http://www.agnld.uni-potsdam.de/~metz/index.html)

Biomembranes are exceptionally crowded with proteins with typical protein-to-lipid ratios being around 1:50–1:100. Protein crowding has a decisive role in lateral membrane dynamics as shown by recent experimental and computational studies that have reported anomalous lateral diffusion of phospholipids and membrane proteins in crowded lipid membranes. Based on extensive simulations and stochastic modeling of the simulated trajectories, we here investigate in detail how increasing crowding by membrane proteins reshapes the stochastic characteristics of the anomalous lateral diffusion in lipid membranes. We observe that cor-

related Gaussian processes of the fractional Langevin equation type, identified as the stochastic mechanism behind lipid motion in noncrowded bilayer, no longer adequately describe the lipid and protein motion in crowded but otherwise identical membranes. It turns out that protein crowding gives rise to a multifractal, non-Gaussian, and spatiotemporally heterogeneous anomalous lateral diffusion on time scales from nanoseconds to, at least, tens of microseconds. Our investigation strongly suggests that the macromolecular complexity and spatiotemporal membrane heterogeneity in cellular membranes play critical roles in determining the stochas-

tic nature of the lateral diffusion and, consequently, the associated dynamic phenomena within membranes. Clarifying the exact stochastic mechanism for various kinds of biological membranes is an important step towards a quantitative understanding of numerous intramembrane dynamic phenomena.

■ **J.-H. Jeon, M. Javanainen, H. Martinez-Seara, R. Metzler, and I. Vattulainen:** *Protein crowding in lipid bilayers gives rise to non-Gaussian anomalous lateral diffusion of phospholipids and proteins;* *Phys. Rev. X* 6, 021006 (2016)



**Figure 1:** Snapshots of the membrane systems at the end of the respective simulations runs. From left to right: (i) protein-poor membrane composed of 2045 DPPC phospholipids and a single NaK channel protein; (ii) protein-rich membrane system composed of 1600 DPPC lipids and 16 NaK proteins: aggregating system; (iii) protein-rich membrane system composed of 1600 DLPC lipids and 16 NaK proteins: nonaggregating system; (iv) schematic structures of a DPPC phospholipid and a NaK channel protein employed in our coarse-grained simulations. For both DPPC and the NaK channel, the transparent coarse-grained structure is shown on top of the atomistic representation.

## SHAPE AND INNER STRUCTURE OF DNA ORIGAMI IN HARSH IONIC CONDITIONS

PD Dr. Bert Nickel, Prof. Tim Liedl, and Prof. Joachim Rädler (LMU München, Physics Department)

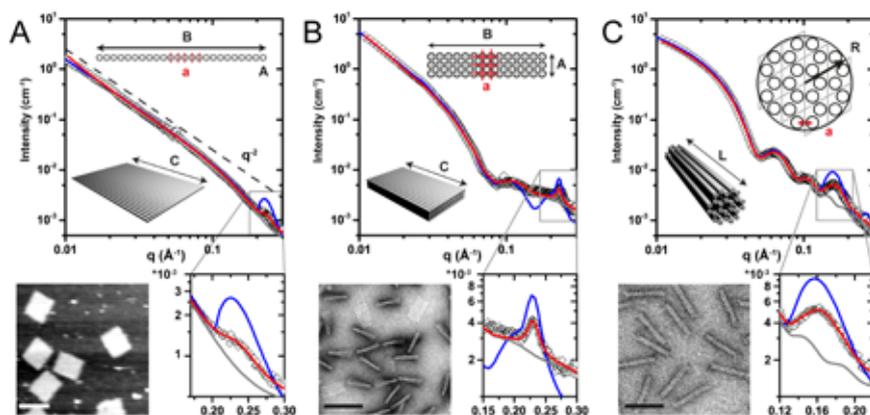
■ [www.softmatter.physik.lmu.de](http://www.softmatter.physik.lmu.de)

Scaffolded DNA origami nanostructures enable the rational design of nearly arbitrarily shaped objects. The assembly of the structures is accomplished by subjecting the DNA supplied with divalent or monovalent salts to screen the negative charge of the DNA during annealing ramps. This imposes constraints on the stability of the resulting structures concerning buffer conditions and temperature. The established methods for characterization of these structures such as transmission electron

microscopy (TEM) operate in vacuum and in contact with a substrate. Small angle X-ray scattering (SAXS) can provide exclusive information about the structures of DNA origami objects in their natural environment in order to probe structural integrity.

In an article published in *Nanoletters* we reported on high precision measurements of overall shape and inter-helical distance of DNA origami structures in solution using synchrotron SAXS. Sheet-, brick-, and

cylinder-shaped DNA constructs were determined with angstrom resolution from fits to the scattering profiles (Figure 1). Furthermore, we tested the cylinder-shaped structure with different salt concentrations and temperature. A key observation is that with decreasing divalent salt concentration, an electrostatic swelling of both shape cross section and inter-helical DNA spacing of the DNA origami structure before it completely disassembles. The maximum swelling is about 10%, in striking analogy to the Lindemann-criterion for the melting of solids. In contrast, with increasing temperature, the cylinder-shaped structures show no thermal expansion in a wide temperature window before they abruptly melt above 50 °C. Hence SAXS revealed distinct effects on the inter-helical spacing in DNA origami in solution under varying electrostatic conditions and hence will be useful to improve assembly protocols and assessment of strains and stresses within the DNA nanostructures.



**Figure 1:** Small angle X-ray scattering intensity of three different types of DNA origami structures in solution with corresponding model, lattice structure (with unit cell) and AFM or TEM image: (A) one-layer sheet, (B) three-layer block with square lattice design, and (C) 24-helix bundle with honeycomb lattice design. Three different model fits are shown for each intensity plot. The geometric model takes only the overall shape—that is, sheet, block, or cylinder—into account (gray lines). A model treating the double helices as rigid cylinders predicts the existence and position of a peak corresponding to inter-helical distance but overestimates the peak's intensity (blue lines). The combination of the geometric model with a Lorentzian peak attributed to the inter-helical arrangement reproduces the scattering intensity with high accuracy (red lines). Scale bars: 100 nm. Reprinted with permission from *Nano Lett.*, 2016, 16 (7), pp 4282–4287. Copyright 2016 American Chemical Society.

■ **S. Fischer, C. Hartl, K. Frank, J. O. Rädler, T. Liedl, and B. Nickel:** *Shape and Interhelical Spacing of DNA Origami Nanostructures Studied by Small-Angle X-ray Scattering; Nano Lett.* 16 (7), 4282–4287 (2016)

## EXPLAINING THE NMR SPECTRUM OF THE ACTIVE SITE OF PHOTOACTIVE YELLOW PROTEIN AS A DYNAMIC EQUILIBRIUM OF HYDROGEN-BOND CONFORMERS

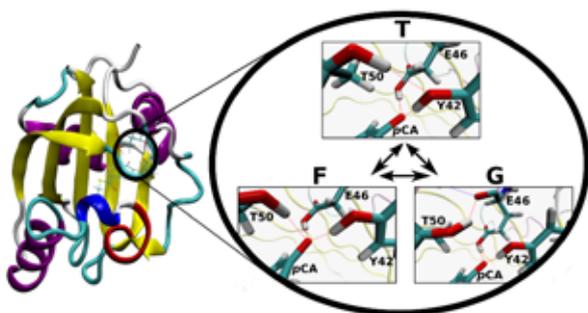
Prof. Christian Ochsenfeld (LMU München, Chemistry Department)

■ [www.cup.uni-muenchen.de/pc/ochsenfeld](http://www.cup.uni-muenchen.de/pc/ochsenfeld)

Photoactive Yellow Protein (PYP) is a small bacterial photoreceptor to short-wavelength light. In addition to its photocycle, which is still an ongoing area of research, the hydrogen bond network of PYP's active site has been the subject of much controversy in the literature. The first neutron diffraction structure showed a very short hydrogen bond between the chromophore, *p*-coumaric acid (pCA), and a nearby glutamate residue (glutamate-46), in which the proton was found at the approximate midpoint of the bond. This unusual geometric arrangement was described as a low barrier

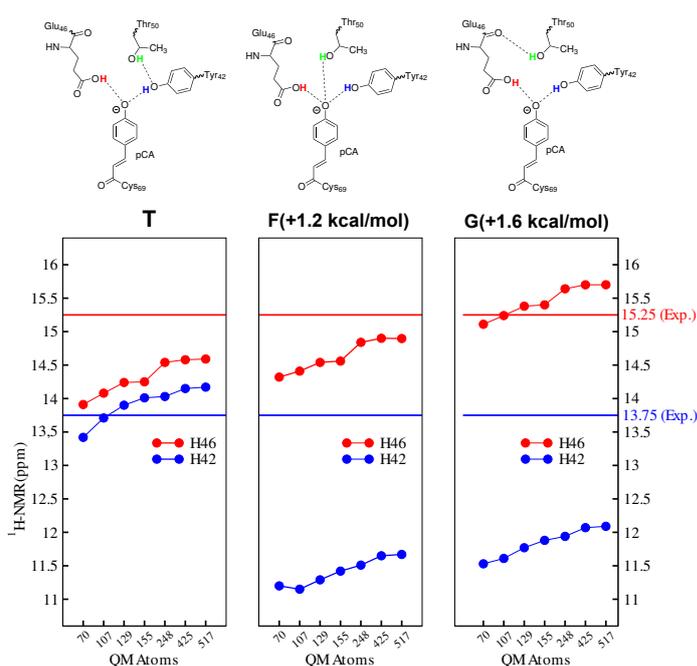
hydrogen bond (LBHB). This discovery prompted both theoretical and experimental investigations of the hydrogen bond network surrounding the active site. A major focus of these investigations was the NMR properties of the active site, as the proposed LBHB has a characteristic, far downfield NMR shift. However, theoretical and experimental NMR studies proved difficult to reconcile, and some of the results were even qualitatively contradictory. Our study using detailed quantum chemical calculations revealed the existence of three conformers of the hydrogen

bond network separated energetically by less than 2 kcal/mol, as well as a rapid exchange mechanism connecting all three. These conformations differ by the rotation of a single threonine residue facing the chromophore, which influences the geometries of the hydrogen bonds between the chromophore, glutamate-46, and tyrosine-42. It is only by combining the calculated NMR shifts of each individual conformer in an energetically weighted scheme that the experimental observations can be qualitatively and quantitatively explained.



**Figure 1:** The active site of Photoactive Yellow Protein is characterized in solution by the rapid interchange of three hydrogen bond conformers.

**Figure 2:** Convergence behavior of the QM/MM calculated NMR shifts of the pCA-glutamate-46 (red), and pCA-tyrosine-42 (blue) protons with respect to the size of the QM region. The data shows that no single conformer is able to explain the experimental NMR spectrum. By taking the energy-weighted average NMR shifts over all three, we obtain NMR shifts of 14.6 and 13.7 ppm for the glu-46 and tyr-42 protons, in excellent agreement with the experiment.



By taking these findings into account, we were thus able to offer a more complete description of PYP's behavior under solution conditions, and provide a first thorough theoretical explanation for the origins of the experimentally observed NMR spectrum. Our findings further

indicate that all three conformers have similar vertical electronic excitation energies, which implies that PYP's photocycle may have multiple starting points.

■ **P. J. Taenzler, K. Sadeghian, C. Ochsenfeld:** *A dynamic equilibrium of three hydrogen-bond conformers explains the NMR spectrum of the active site of photoactive yellow protein;* J. Chem. Theory Comput., 12, 5170 (2016)

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## DIRECT COMPARISON OF PHYSICAL PROPERTIES OF BACILLUS SUBTILIS NCIB 3610 AND B-1 BIOFILMS

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**Prof. Oliver Lieleg (TU München, Institute of Medical Engineering)**

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Many bacteria form surface-attached communities known as biofilms. Due to the extreme resistance of these bacterial biofilms to antibiotics and mechanical stresses, biofilms growing on pipes or medical catheters cause severe problems in healthcare and industry. It is therefore of great interest to understand which biomolecules that are constituting the biofilm matrix the individual bacteria are encased in, cause e.g. the mechanical sturdiness of a bacterial biofilm. Investigating the model bacterium *Bacillus*

*subtilis*, the researchers show that particular surface properties of *B. subtilis* biofilms, e.g. the surface roughness and surface elasticity of one-day old *B. subtilis* NCIB 3610 biofilms, are strongly affected by the surface layer protein BslA. Furthermore, they demonstrated that a different strain, *B. subtilis* B-1, is protected from ethanol induced changes in the biofilm's bulk stiffness and that this protective effect can be transferred to NCIB 3610 biofilms by the sole addition of  $\gamma$ -polyglutamate to growing NCIB 3610

biofilms. Taken together, this study demonstrates the importance of specific biofilm matrix components for distinct physical properties of *B. subtilis* biofilms.

■ **S. Kesel, S. Grumbein, I. Gümperlein, M. Tallawi, A-K. Marel, O. Lieleg and M. Opitz:** *Direct comparison of physical properties of Bacillus subtilis NCIB 3610 and B-1 biofilms.* Applied and Environmental Microbiology. 82(8):2424-2432 (2016)

## CONTROL OF LIPID RAFTS WITH PHOTOSWITCHABLE CERAMIDES\*

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■ [www.biochem.mpg.de/en/rd/schwille](http://www.biochem.mpg.de/en/rd/schwille)

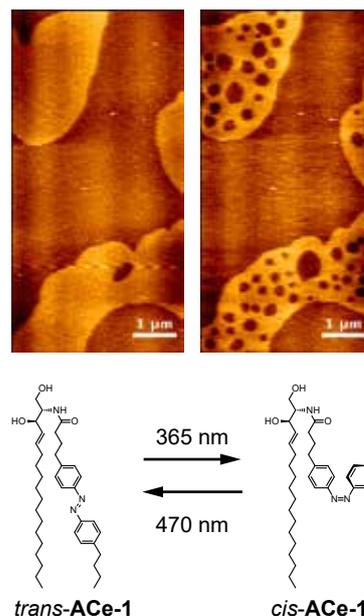
Prof. Dirk Trauner (LMU München, Chemistry Department)

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Ceramide is a pro-apoptotic sphingolipid with unique physical characteristics. Often viewed as a second messenger, its generation can modulate the structure of lipid rafts. We prepared three photoswitchable ceramides, ACes, which contain an azobenzene photoswitch allowing for optical control over the N-acyl chain. Using combined atomic force and confocal fluorescence microscopy, we demonstrate that the ACes enable reversible switching of lipid domains in raft-mimicking supported lipid bilayers (SLBs). In the trans-configuration, the ACes localize into the liquid-ordered (Lo) phase. Photoisomerization to the cis-form triggers a

fluidification of the Lo domains, as liquid-disordered (Ld) "lakes" are formed within the rafts. Photoisomerization back to the trans-state with blue light stimulates a rigidification inside the Ld phase, as the formation of small Lo domains. These changes can be repeated over multiple cycles, enabling a dynamic spatiotemporal control of the lipid raft structure with light.

■ **J. A. Frank, H. G. Franquelim, P. Schwille and D. Trauner:**  
*Optical Control of Lipid Rafts with Photoswitchable Ceramides;*  
*Journal of the American Chemical Society*, 10.1021/jacs.6b07278 (2016)



## TUNING THE OPTICAL PROPERTIES OF PEROVSKITE NANOPATELETS THROUGH COMPOSITION AND THICKNESS BY LIGAND-ASSISTED EXFOLIATION\*

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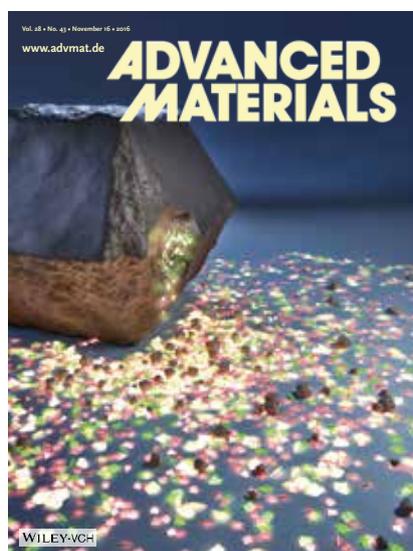
Hybrid organic/inorganic perovskites have become a very hot topic through an unprecedented improvement in solar to electrical conversion efficiencies in thin film solar cells. Additionally, perovskite nanocrystal-based LEDs and lasers have recently been rapidly gaining more interest due to the high tunability of the emission wavelength and excellent quantum yields of over 90%.

In this project, a versatile approach for the fabrication of colloidal 2D perovskite nanoplatelets (NPLs) via a ligand-assisted liquid-phase exfoliation technique is demonstrated. The absorption and emission can be tuned through the entire visible spectrum (395–770 nm) by using combinations of halide ions (Cl<sup>-</sup>, Br<sup>-</sup>, or I<sup>-</sup>). Moreover, through centrifugation bulk-like NCs are separated from NPLs, which are confined strongly in one dimension, leading to quantum confinement effects. This gives additional flexibility for fine-tun-

ing the optical properties of perovskite NCs. Overall quantum efficiencies of the perovskite NCs are quite high, peaking at around 70%. Additionally, the dispersions are extremely stable, hardly changing over months, when stored in the dark in ambient conditions. Focusing on the iodide-containing perovskites, suspensions of NPLs with a specific thickness down to a single perovskite monolayer were prepared through centrifugation. This enabled an investigation of the dependence of several optical and electronic properties of the NPLs on their thickness. Not only do they show large exciton binding energies of a few hundred meVs, which increase with decreasing thickness of the NPLs. Moreover they exhibit an increase in the radia-

tive decay rates for decreasing NPL thickness, analogous to epitaxial III-V semiconductor quantum wells at low (< 10K) temperatures. Not only should NCs produced in this manner lead to applications for light emission, but also permit further studies on optical and electronic properties of perovskites, enabling important insights into this fascinating material.

■ **V. A. Hintermayr, A. F. Richter, F. Ehrat, M. Döblinger, W. Vanderlinden, J. A. Sichert, Y. Tong, L. Polavarapu, J. Feldmann, A. S. Urban:** *Tuning the Optical Properties of Perovskite Nanoplatelets through Composition and Thickness by Ligand-Assisted Exfoliation; Advanced Materials* 28 (43), 9478–9485 (2016)



**Figure 1:** Organic/inorganic halide perovskite nanoplatelets are exfoliated from microcrystals of the same material through ligand-assisted liquid-phase tip sonification. The nanoplatelets are hundreds of nanometers large but extremely thin, down to a single-crystal-unit monolayer. Due to the strong quantum confinement, the transition energy of the nanoplatelets is shifted into the visible, leading to brightly fluorescing nanoplatelets of various colors. Image by Cristoph Hohmann (Nanosystems Initiative Munich), courtesy of Advanced Materials.

## MECHANICS AND STRUCTURE OF MOLECULAR MOTOR PROTEINS

Prof. Claudia Veigel (LMU München, Medical Faculty)

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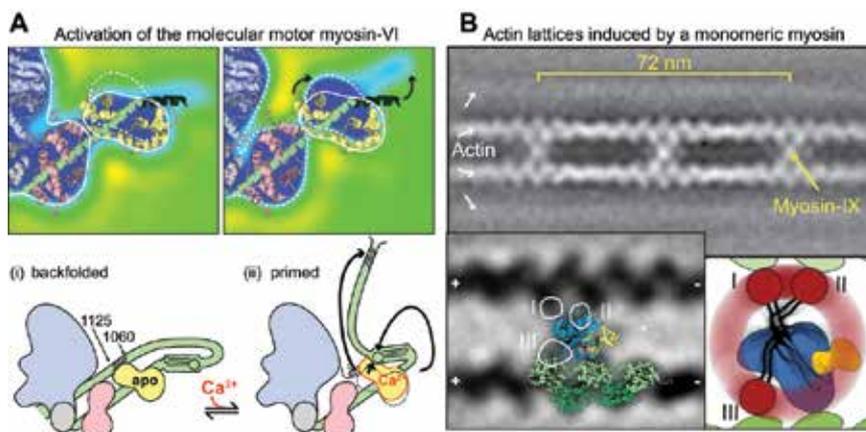
(a) Calcium can mobilize and activate myosin-VI. The timing of motor protein activation is central to a broad range of cellular motile processes including endocytosis, cell division and cancer cell migration. The cytoskeletal motor protein myosin-VI is central to these processes. Combining single particle electron microscopy, fluorescence spectroscopy and motility assays the authors discovered that calcium is a cellular switch that directs the structural rearrangement of this molecular motor from a dormant, inactive state at low calcium to a cargo-binding non-motile state at high calcium. The return to low calcium generates either car-

go-bound motors that are now able to translocate to the centre of the cell, or refolded inactive motors ready for the next cellular calcium flux. With this mechanism cellular calcium fluxes can induce waves of localised motor activity.

(b) Self-organization of actin networks by a monomeric myosin. Myosin class IX plays a critical role in acto-myosin networks that are required for cell polarisation and collective cell migration during morphogenesis and development. Using quantitative super-resolution fluorescence microscopy, fluorescence spectroscopy and single particle electron microscopy the authors discovered that myo-

sin-IX assembles actin filaments into highly ordered lattices of parallel filament polarity connected by myosin-IX in distinct structural conformations and at a repeat distance of precisely 36 nm across the network. It emerges that these actin lattices induced by myosin-IX introduce orientated tracks with regularly spaced platforms for localised signalling protein activity during cell polarisation and collective cell migration.

■ **D. Saczko-Brack, E. Warchol, B. Rogez, M. Kröss, S.M. Heissler, J.R. Sellers, C. Batters and C. Veigel:** *Self-organization of actin networks by a monomeric myosin*; Proc Natl Acad Sci USA 113, E8387-E8395 (2016)



**Figure 1 (A)** The modelled high-resolution structure of the known elements of the molecular motor myosin class VI were overlaid onto an electron microscopic class average. The data reveal a novel molecular mechanism how myosin-VI can be transformed from a dormant back-folded and inactive state, to an unfolded cargo-binding and primed, and finally to a mechanically active state in the cell. **(B)** We discovered that the molecular motor myosin class IX (with its unique flexible insert (red) at the catalytic domain (blue)) can induce the formation of extended actin lattices by forming crosslinks between filaments with parallel polarity. The motor can adopt three different conformations, crosslinking two filaments (I, II) or binding in an inchworm fashion to a single filament. This is the first example of actin lattices induced by a monomeric cytoskeletal motor.

**C. Batters, D. Brack, H. Ellrich, B. Averbek and C. Veigel:** *Calcium can mobilize and activate myosin-VI*; Proc Natl Acad Sci USA 113, E1162-E1169 (2016)  
**Commentary on this paper:** Calcium gets myosin-VI ready for work. Proc Natl Acad Sci USA 113, 2325-2327 (2016).

## FOLATE RECEPTOR TARGETED SI RNA NANOPARTICLES FOR TUMORAL EGLIN 5 GENE SILENCING AND CURE OF MICE\*

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Successful application of RNAi-based cancer therapy depends upon efficient intracellular delivery of siRNA and effective knockdown of targeted genes. For treatment of folate receptor-expressing tumors, a series of sequence-defined oligomers were synthesized, which include a cationic oligoaminoamide core and polyethylene glycol (for shielding surface charges) coupled to folic acid or, alternatively, the antifolate drug methotrexate (MTX). MTX may act both as targeting ligand for tumor uptake and as an anticancer agent, as it is toxic by blocking de novo thymidylate and purine synthesis in cancer cells.

Antitumoral Eglin-5 (EG5) siRNA together with the targeted oligomers form small nanoplexes with a hydrodynamic diameter of only 6.5 nm (Figure 1). Intratumoral administration of MTX-based polyplexes in KB carcinoma-bearing mice showed significantly prolonged survivals and also 50% cures of tumor mice.

To increase the siRNA polyplex stability for systemic delivery, the physicochemical properties of polyplexes were optimized by combination of PEGylated folate-conjugated oligomers and 3-arm thiol-oligomers. These targeted combinatorial polyplexes (TCPs) are homogeneous

spherical particles with size of around 100 nm favorable for intravenous administration, reducing the EG5 gene expression in distant subcutaneous L1210 lymphocytic leukemia tumors. In sum, multifunctional chemically precise siRNA carrier systems display potential for in vivo tumor targeted gene silencing and RNAi-based cancer therapy.

■ **D.J. Lee, E. Kessel, D. Edinger, D. He, P.M. Klein, L. Voith von Voithenberg, D.C. Lamb, U. Lächelt, T. Lehto, E. Wagner:** *Dual antitumoral potency of EG5 siRNA nanoplexes armed with cytotoxic bifunctional glutamyl-methotrexate targeting ligand;* *Biomaterials* 77, 98-110 (2016)

**D.J. Lee, D. He, E. Kessel, K. Padari, S. Kempster, U. Lächelt, J.O. Rädler, M. Pooga, E. Wagner:** *Tumoral gene silencing by receptor-targeted combinatorial siRNA polyplexes;* *J. Control. Release* 244, 280-291 (2016)

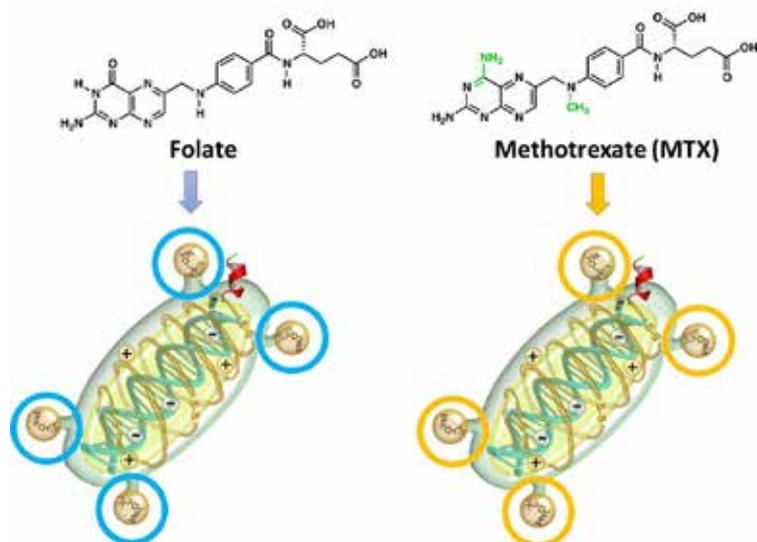


Figure 1: siRNA nanoplexes

## CLASSICAL STÜCKELBERG INTERFEROMETRY OF A NANOMECHANICAL TWO-MODE SYSTEM

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Prof. Jörg P. Kotthaus (LMU München, Physics Department)

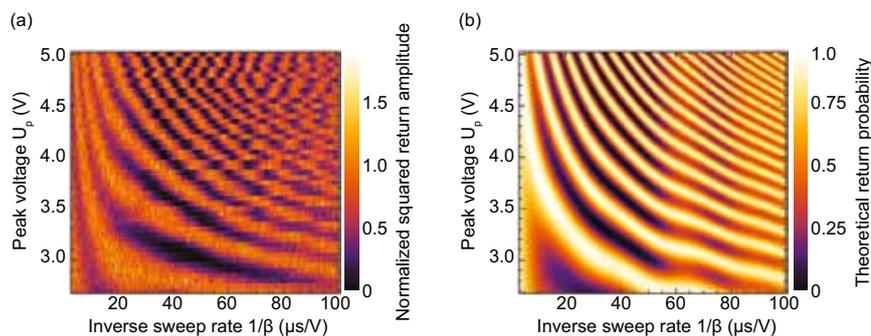
■ [www.nano.physik.uni-muenchen.de](http://www.nano.physik.uni-muenchen.de)

In the past years, quantum-classical analogies have attracted considerable interest. One example are interfering waves, which occur in systems with sufficiently long coherence. Interference phenomena hence appear both in a quantum-mechanical and in a classical context. One prominent example is Stückelberg interference, which arises under a double passage through an avoided level crossing and which has previously been understood exclusively as a pure quantum effect. Recently, a classical analog of Stückelberg interferometry has been demonstrated using a high Q nanomechanical system. The two coherent classical states are represented by two strongly

coupled nanomechanical resonator modes, the out-of-plane and the in-plane fundamental flexural mode of a silicon nitride nanostring, with lifetimes in the millisecond regime at 300 K. Dielectric frequency control allows tuning the modes through their avoided crossing. Initialization of the out-of-plane mode followed by the application of a triangular voltage ramp realizes the characteristic double passage through the avoided crossing of a Stückelberg experiment. Self-interference of the mechanical modes is a consequence of the difference in phase picked up along the two branches of the avoided crossing. Variation of both the peak voltage of the voltage ramp and the ramp rate

yields an interference pattern, which is well described by Stückelberg interferometry. Moreover, a thorough theoretical analysis reveals that the Stückelberg interference pattern completely coincides for the quantum mechanical and the classical version of the problem. Consequently, all possible applications that have been thought of in the context of “quantum” Stückelberg interferometry can now be exploited with “classical” Stückelberg interferometry of distinct macroscopic objects, such as the presented strongly coupled modes of a nanomechanical string resonator.

■ **M. J. Seitner, H. Ribeiro, J. Kölbl, T. Faust, J. P. Kotthaus, E. M. Weig:** *Classical Stückelberg interferometry of a nanomechanical two-mode system*; *Phys. Rev. B* 94, 245406 (2016)



**Figure 1:** Classical Stückelberg interferometry in experiment and theory. **(a)** Experimental data showing color-coded normalized squared return amplitude vs inverse sweep rate and peak voltage. **(b)** Theoretical model displaying color-coded theoretical return probability vs inverse sweep rate and peak voltage for the equivalent data range. The theory is calculated with a single set of parameters extracted from the experiment and contains no free parameters.

## HETEROGENEITIES IN METAL-ORGANIC FRAMEWORKS

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■ [www.wuttkegroup.de](http://www.wuttkegroup.de)

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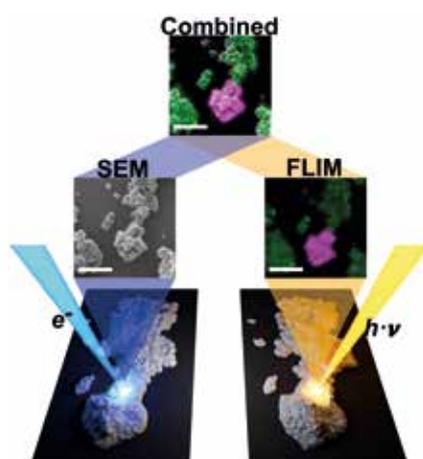
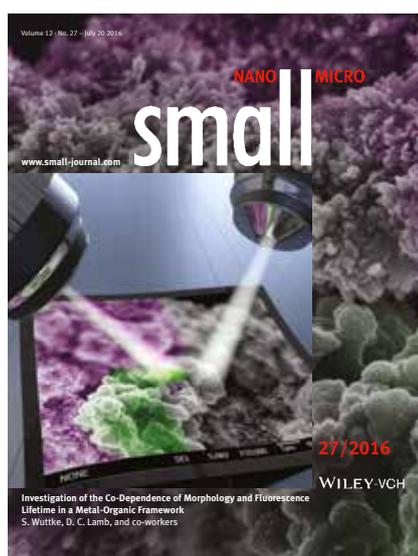
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Metal-organic frameworks (MOFs) are a relatively new class of porous hybrid materials. Due to their exceptionally high surface areas, and their high variability and adaptability, MOFs have attracted considerable attention as potential materials for various applications such as gas storage, separation, catalysis, biomedical applications, or chemical sensors. Most methods employed in these studies yield information about the materials' bulk properties such as crystallinity, surface area, chemical composition, or absorbance. However, they are often not sufficient to investigate

heterogeneities and their distribution within the material. Even for highly crystalline structures, the nanoscopic environment can be very heterogeneous due to differences in crystal size or shape, defects or small variances in molecular composition that do not significantly affect the overall structure. However, these defects and heterogeneities might strongly influence the behavior of the material, such as the catalytic performance, where defects are often the actual active centers.

We tackled this issue of resolving heterogeneities at the nanoscopic level by developed a

new strategy that is based on a combination of scanning electron microscopy (SEM) and fluorescence lifetime imaging microscopy (FLIM). As the fluorescence lifetime of many dyes is very sensitive and selective to their local environment, changes on the nanoscopic level can be detected and even quantified in the lifetime decay of a fluorescence probe. Thus, FLIM can be applied to identify heterogeneities, defects or analytes, while the SEM images provide morphology information on the nanometer scale that cannot be resolved with light microscopy due to the diffraction limit. By combining both techniques, we could distinguish different microscopic species in a MOF and relate their distinct lifetimes with the measured morphologies. Our results illustrate the importance of using microscopy to analyze porous materials (even the "same" material from different batches), since changes of the microscopic structure and morphology influence the performance (in this case, fluorescence lifetime), without affecting many of the routinely measured bulk properties. This approach can be adapted and applied to a wide variety of materials and sensors, and provide a deeper understanding



**Figure 1 Left:** Cover image. Image: C. Hohmann (NIM). **Right:** Schematic illustration of the novel correlative SEM/FLIM approach. Comparative analysis of the same regions imaged with both techniques reveals correlations between morphology and fluorescence lifetime. The scalebars correspond to 10  $\mu\text{m}$ .

of local heterogeneities and functionalities that are not resolvable with current methods.

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[Front Cover]



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