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Channels and Bridges to the Nanoworld

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Content

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Invited Talks

Molecular choreography on a tightrope: a single-molecule view of DNA replication

Antoine van Oijen

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Advances in optical imaging and fluorescence spectroscopy have made it possible to circumvent the classical diffraction limit of light and visualize living systems at the nanometer scale. Our group is interested in combining these approaches with novel molecular manipulation techniques to study biological processes at the single-molecule level. By recording 'molecular movies' of individual enzymes we hope to gain new insight into reaction dynamics and mechanisms. In a biological context, most of these enzymes function in concert with other enzymes in multi-protein complexes, so an important direction is the utilization of single-molecule techniques to unravel the orchestration of large macromolecular assemblies. I will present our single-molecule studies on DNA replication, the duplication of genomic DNA prior to cell division. This process is supported by a large, multi-protein complex containing a number of different enzymatic activities whose coordination is still poorly understood. I will discuss recent results of single-molecule studies of replication in bacterial and eukaryotic systems, both *in vitro* and *in vivo*. By combining the mechanical stretching of individual DNA molecules with the fluorescence observation of individual proteins, we visualize the dynamic behavior of replication complexes during replication *in vitro* and unravel mechanistic working principles that challenge aspects of the existing textbook view of replication. Further, I will present imaging studies that aim to visualize in live cells the interplay between DNA replication and repair at the single-molecule level.

Carbon Nanostructures as Functional Multitalents – Sensing, Catalysis, Drug Delivery, Electronics

Klaus Müllen

Max Planck Institute for Polymer Research, 55128 Mainz, Germany

We introduce carbon nanostructures of different size, dimensionality and structural complexity. Dendrimers made from twisted and interlocked benzene rings constitute shape-persistent nanoparticles allowing perfect site definition of functional groups. This affords light harvesting complexes, receptors for guest up-take and sensing, drug delivery vehicles as well as single-molecule rotors. On the other hand, these dendrimers serve as 3D-precursors for the bottom-up synthesis of nanographenes and graphene nanoribbons (GNRs). Graphene is praised as a multifunctional "wonder" material and rich playground for physics. Above all, however, it is a 2D-polymer and thus a task for materials synthesis. Thereby "conventional" GNR-synthesis can be compared with a surface-bound synthesis under in-situ control by scanning tunneling spectroscopy. We then compare our "bottom-up" precision synthesis starting from dendrimers with "top-down" protocols starting from graphite. The available toolbox of fabrication methods provides access to an enormous breadth of materials for batteries, supercapacitors, oxygen reduction catalysts and semiconductors.

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Nature Chemistry 2014, 6, 126

Nature Communications 2014, DOI:10.1038/ncomms5973

Nature Nanotechnology 2014, 9, 896

Nature Communications 2014, DOI:10.1038/ncomms5253

Light-induced cation exchange for copper sulfide based CO_2 reduction

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Copper (I) based catalysts, such as Cu_2S, are considered to be very promising materials for photocatalytic CO_2 reduction.[1] A common synthesis route for Cu_2S via cation exchange from CdS nanocrystals requires Cu (I) precursors, organic solvents and neutral atmosphere, but these conditions are not compatible with in-situ applications in photocatalysis. We report a novel cation exchange method in which we harness the reducing potential of photoexcited electrons in the conduction band of CdS nanocrystals to fabricate Cu_2S nanorods from CdS using Cu^{2+} precursors. In contrast to other cation exchange methods, this photoinduced process can proceed in an aqueous environment and under aerobic conditions, yet preserves the shape of the original crystals and enables complete conversion of CdS to copper sulfide.[2] We show that the as-prepared Cu_2S nanorods can be efficiently used for the reduction of CO_2 to carbon monoxide and methane, achieving formation rates of 3.02 µmol $h^{-1}g^{-1}$ and 0.13 µmol $h^{-1}g^{-1}$, respectively, and suppressing competing water reduction. The process opens new pathways for the preparation of new efficient photocatalysts from readily available nanostructured templates.

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[2] A. Manzi, T. Simon, C. Sonnleitner, M. Döblinger, R. Wyrwich, O. Stern, J. K. Stolarczyk, J. Feldmann, manuscript submitted, 2015.

tba

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Manipulating light with nanostructures: controlling reflection to chemical imaging

Michael J. Gordon

Dept. of Chemical Engineering, University of California, Santa Barbara

This talk will highlight some of our recent work in bio-inspired photonics and plasmonics related to controlling reflection at interfaces and nanoscale chemical imaging. In the former, an easy, scalable and defect-tolerant surface modification protocol, based on colloidal lithography and plasma etching, was developed to create synthetic 'moth-eye' anti-reflective structures on different surfaces for applications in photon detection and extraction. Large increases in transmission, bandwidth, and omni-directional response were obtained in Si, Ge, and GaAs platforms over the mid- and far-IR spectral regions (2-50+ μm) with performance better than commercial coatings. Effective medium theory and quantitative measurements of transmission, reflection and diffuse scattering were used to understand the 'photon balance' of moth-eye films to investigate how scattering phenomena are affected by moth-eye geometry.

In the materials characterization realm, we are developing hybrid atomic force microscopes that manipulate light below the diffraction limit ($\lambda/2$) to locally "image" surface structure and chemistry. Nanometer-scale optical fields are created at the apex of an optical antenna tip when laser light excites plasmons (i.e., collective oscillations of free electrons) in the tip material. The resulting field is then used to directly probe molecular vibrations of the surface by way of inelastic light scattering (Raman spectroscopy). Since the optical field enhancement by the tip is nanoscale, vibrational spectroscopy and chemically-specific surface imaging below the diffraction limit can be accomplished.

Cell-free genetic systems for the construction of cellular mimics

Sheref Mansy

Centre for Integrative Biology (CIBIO) at the University of Trento, Italy

Cell-free transcription–translation reactions are typically unresponsive to analytes and are constructed with strong transcriptional promoters and ribosome binding sties to maximize the production of gene products. Such an approach is successful for the expression of a single protein but not well tuned to building more complex systems that integrate with the surrounding environment in a manner similar to that of a living cell. To this end, we have determined the influences of mRNA and protein expression on multigene construct performance and used the resulting genetic systems to construct cellular mimics capable of responding to the environment and communicating with natural, living cells.

Electrostatically tunable metasurfaces for controlling optical wavefronts and thermal emission

Victor Brar

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Metasurfaces composed of sub-wavelength artificial structures have shown potential for extraordinary light-manipulation. By controlling the phase fronts of optical waves, these structures have allowed for the development of ultrathin optical components such as lenses, filters and waveplates, and they have provided a pathway to create holograms over a broad range of the electromagnetic spectrum. Structures developed to date, however, are static and do not allow for post-fabrication control of the metasurface properties. We have created and investigated metasurfaces with active elements that incorporate indium tin oxide (ITO) and graphene in their structure. In these devices, the optical resonances of normal metal patch antennas interact with the carrier density dependent permittivity of the ITO/graphene to enable control of the antenna resonance frequency and amplitude. This process facilitates the realization of sub-wavelength, gate tunable phase arrays in the infrared that can be operated at high frequencies. These surfaces also exhibit variable absorbtivity and emissivity, properties that are typically viewed as fixed material parameters. We leverage this effect to demonstrate electrostatic control of the thermal emission spectrum from a surface at fixed temperature. The operation of these metasurfaces for beam steering applications and as low-cost mid-IR sources will be discussed, along with their inherent advantages and disadvantages over conventional LCD technology.

Mechanisms of membrane transport: a single-molecule view on ABC importers

Thorben Cordes

University of Groningen, The Netherlands

Membrane transporters are vital to any living system and involved in the translocation of a wide variety of substrates. Despite their importance, all proposed molecular models for transport are based on indirect evidence due to the inability of classical biophysical and biochemical techniques to visualize dynamic structural changes. My group has recently started to use single-molecule fluorescence microscopy to characterize conformational states and changes in ATP-binding cassette (ABC) transporters in vitro to directly observe how different steps in transport are coordinated.

My talk will focus on the homodimeric GlnPQ complex, a bacterial ABC-importer, possessing two different substrate-binding proteins (SBDs) per single translocator. To decipher how conformational changes within the different subdomains drive transport, we use a combination of single-molecule methods and classical biochemical techniques (calorimetry and uptake assays). We demonstrate by single-molecule Förster resonance energy transfer (FRET) that the two SBDs intrinsically transit from open to closed ligand-free conformation, and the proteins capture their amino acid ligands via an induced-fit mechanism. High-affinity ligands elicit transitions without changing the closed-state lifetime, whereas low-affinity ligands dramatically shorten it. We show that SBDs in the closed state compete for docking onto the translocator, but remarkably the effect is strongest without ligand. We find that the rate-determining steps for translocation depend on the SBD and the amino acid transported. We conclude that the lifetime of the closed conformation controls both SBD docking to the translocator and substrate release.

Tailor-made synthesis and ligand design for the use of nanocrystals in materials- and life science applications

Horst Weller

Department of Chemistry, University of Hamburg, Center for Applied Nanotechnology Hamburg (CAN), Interdisciplinary Nanoscience Center Hamburg (INCH), The Hamburg Center for Ultrafast Imaging (CUI), Germany

We report on the precision synthesis of CdSe/CdS/ZnS core-shell-shell nanocrystals using a preparative flow reactor. Experimental design is used to determine the crucial parameters and their influence on particle growth and size distribution.

In the second part of the talk, we will present applications of nanocrystals. In particular, we will report on the development of quantum dot quantum rod particles with fluorescence quantum efficiencies close to unity and applications in lighting and display technology. For biomedical applications we will present a biocompatible encapsulation technique based on amphiphilic poly(isoprene-*block*-ethylene oxide) (PI-*b*-PEO) diblock copolymers. We varied block lengths, structure and functional terminal end groups and investigated the effect on unspecific uptake. Fluorescence quenching experiments with encapsulated quantum dots show that best behavior in respect to unspecific cellular uptake is realized in those systems, in which the polymer shell yielded best protection against quenching molecules from the surrounding medium. Combination of micelle encapsulation with block copolymers and seeded emulsion polymerization finally leads to biolables for which unspecific uptake could be almost completely suppressed even under in-vivo conditions. We present various techniques for bio-conjugation with recognition molecules and show examples for specific cell and tissue targeting. In-vitro and in-vivo fluorescence and MRI data will be discussed.

Breaking detailed balance at the mesoscale in active biological systems

Chase Broedersz

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Systems in thermodynamic equilibrium are not only characterized by time-independent macroscopic properties, but also satisfy detailed balance: transitions between microscopic configurations are perfectly balanced. Living systems function out of equilibrium and are characterized by directed fluxes through chemical states, which violate detailed balance at the molecular scale. Here we demonstrate how breaking of detailed balance is manifest in dynamics at mesosopic scales. The periodic beating of an isolated flagellum from *Chlamydomonas reinhardtii* exhibits probability flux in the phase space of shapes. With a model, we show how the breaking of detailed balance can be quantified in stationary, non-equilibrium stochastic systems in the absence of periodic motion. We further demonstrate that primary cilia of epithelial cells break detailed balance, owing to activation by the cytoskeletal cortex. Finally, we will discuss how this analysis of violations of detailed balance provides a general tool to identify non-equilibrium dynamics in cells and tissues.

Ligand-gated ion channels: From 3D structure to transmembrane signaling

Horst Vogel

Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland

Neurotransmitter-gated ion channels of the Cys-loop receptor family mediate fast neurotransmission throughout the nervous system. The molecular processes of neurotransmitter binding, subsequent opening of the ion channel and ion permeation remain poorly understood. Here we present recent results of high-resolution X-ray crystallography, single particle imaging, and molecular modeling studies of a mammalian Cys-loop receptor, the mouse serotonin 5-HT3 receptor. We revealed at atomic detail how neurotransmitter binding on the extracellular domain of the 5-HT3 receptor induces sequential conformational transitions in the receptor opening a transmembrane ion channel: Agonist binding first induced distinct conformational fluctuations of particular side chains in the highly conserved ligand binding cage, followed by tilting-twisting movements of the extracellular domain which coupled to the transmembrane TM2 helices to open the hydrophobic gate and forming a continuous transmembrane water pathway. The structural transitions in the receptor's transmembrane part finally coupled to the intracellular region opening passages for ion release. The details of structural transitions of the 5-HT3 receptor deliver important insights for understanding the operating mechanism of mammalian Cys-loop receptors.

G. Hassaine et al., Nature 512 (2014) 276

Thermoplasmonic control of chemical reactions and cell function at the nanoscale

Theo Lohmüller

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Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany

Light absorbed by plasmonic nanoparticles is very efficiently converted into heat: Temperatures of several hundred degrees centigrade can be reached within a few nanoseconds when a gold nanoparticle is irradiated with intense light at its plasmon resonance frequency. Individual particles can thus be used as fine tools to apply heat to only a small area. Gold nanoparticles, however, are at the same time subject to optical forces when they are irradiated with a focused laser beam which renders it possible to optically manipulate or trap them in two and three dimensions.

In this talk, I am going to present how plasmonic heating and optical manipulation of gold nanoparticles can be employed to control chemical reactions or biological systems with nanoscale resolution and discuss further applications in material science and biomedicine.

Tuesday, September 22 (afternoon session 1, 2:15-3:00 pm)

Organic electronics: fundamentals and applications of organic field-effect transistors in flexible displays

Thomas Weitz

Field-effect transistor systems, BASF SE, 67056 Ludwigshafen, Germany

Semiconducting materials are an integral part of everyday electronic circuits. Conventional electronics is based on silicon as semiconductor and therefore can be fabricated only on rigid substrates such as glass. Organic semiconductors on the contrary enable plastic-based flexible circuits and displays.

This talk will cover basics on why organic materials enable flexible field-effect transistors and show state-of-the art materials and transistor fabrication techniques. For efficient electronics both high-performance electron- and hole-conducting organic semiconductors are required. I will show some details on an electron conducting semiconductor and discuss novel findings on temperature dependent charge transport in this system. We have found, that the closer charge carriers are confined to the dielectric / semiconductor interface, the lower the electrical performance (expressed in terms of the charge carrier mobility) of the system. These observations are consistent with lattice imperfections in the semiconductor layer in close proximity to the dielectric surface. I will discuss implications of this finding for future device design.

Tuesday, September 22 (afternoon session 2, 5:00-6:30 pm)

Manipulating light, heat and forces at the nanoscale with metallic nanoparticles

Fernando Stefani

Centro de Investigaciones en Bionanociencias (CIBION), Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET)
Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires

Metallic nanoparticles present collective resonances of their electrons at optical frequencies (plasmon resonances), which depend strongly on the composition, shape and near environment and are accompanied by strong scattering and absorption of light. I will show experiments where the interaction of light with metallic nanoparticles enables not only the control light, but also of heat and forces at the nanoscale. I will include our latest results on control of photobleaching, biosensing based on photothermal fluorescence quenching and optical printing connected nanoparticles.

Polymer mechanics across the force regimes

Omar Saleh

Materials Department, University of California Santa Barbara

The elastic response of a single polymer can explain certain material properties, including the thickness of polymer brushes and the mechanics of gels; in turn, these material properties have a variety of biological analogies, such as to the brush-like pericellular matrix surrounding certain cells. More fundamentally, the force-extension relation of a polymer can be predicted theoretically, making it possible to probe the structure of a polymer by measuring its elastic response. This works in a manner similar to scattering: just as scattering at a wave vector q gives information on structure at a length scale 1/q, the elastic response under applied tension f gives information on structure at a length scale $x \sim kT/f$. Thus, in exact analogy to low-angle scattering, low-force elastic measurements are needed to probe the interesting long-range structure of polymers. I will discuss the basic physics of low-force elasticity, and present our experiments on various polymers that validate the power of low-force elastic measurements. I will then focus on the role of electrostatics in modulating the elasticity of charged biopolymers, including single-stranded nucleic acids and hyaluronic acid. This data indicates a need to move beyond classic models of polymer physics (e.g. worm-like chain models); I will discuss progress in formulating such models.

TRP channel structures by single particle cryo-EM - from blob-ology to atomic structures

Yifan Cheng

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As a versatile tool in structural biology, single particle electron cryo-microscopy (cryo-EM) has been used to determine the three-dimensional (3D) structures of proteins and macromolecular complexes without the need for crystals. However, for many years, the achievable resolution of this technique, particularly for integral membrane proteins, was limited at nanometer to sub-nanometer level. These resolutions, while providing valuable structural information, were insufficient for building de novo atomic models. Recent technological breakthroughs in electron detector technologies have enabled developments of novel techniques in data acquisition and image processing. Together, these novel technologies revolutionized single particle cryo-EM and enabled atomic structure determinations of a broad range of proteins complexes without the need of crystals. It is now feasible to use single particle cryo-EM to determine structures of challenging protein complexes, particularly for integral membrane proteins.

The Transient Receptor Potential (TRP) ion channel is a large and functionally diverse superfamily, second only to the potassium channels. Despite many years' effort to determine crystal structures of TRP channel, the first breakthrough was brought by single particle cryo-EM. This accomplishment was enabled by novel cryo-EM technologies developed during the last few years. In this talk, I will discuss these recent technological advances in single particle cryo-EM, and its applications in determining atomic structures of TRP channels.

Decoding chromatin organization with super-resolution microscopy

Melike Lakadamyali

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Nucleosomes help structure chromosomes by compacting DNA into fibers. Chromatin organization likely plays an important role for regulating gene expression; however, due to the nanometer length scales involved, it has been very difficult to visualize chromatin fibers in vivo. To gain insight into how nucleosomes are arranged in vivo, we combined quantitative super-resolution nanoscopy with computer simulations to visualize and count nucleosomes along the chromatin fiber in single nuclei. Nucleosomes assembled in heterogeneous groups of varying sizes, which we named "clutches," in analogy with "egg clutches". Despite the heterogeneity in clutch size in a given nucleus, strikingly, the median number of nucleosomes and their compaction inside clutches were highly cell type specific. Ground-state pluripotent stem cells had, on average, less dense clutches containing fewer nucleosomes and clutch size strongly correlated with the pluripotency grade of induced pluripotent stem cells. RNA polymerase II preferentially associated with the smallest clutches while the large clutches were enriched in heterochromatin. Our results reveal how the chromatin fiber is formed at nanoscale level and link chromatin fiber architecture to stem cell state.

Big-Data Analytics for Materials Science: Concepts, Challenges, and Hype

Matthias Scheffler

Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

On the steady search for advanced or even novel materials with tailored properties and functions, high-throughput screening is by now an established branch of materials research. For successfully exploring the huge chemical-compound space from a computational point of view, two aspects are crucial. These are (i) reliable methodologies to accurately describe all relevant properties for all materials on the same footing, and (ii) new concepts for extracting maximal information from the big data of materials that are produced since many years with an exponential growth rate.

The talk will address both challenges. In particular, I will present a *Test Set for Materials Science and Engineering* that enables quality control of first-principles calculations. Furthermore, I will demonstrate the possibilities offered by statistical learning theory for big data of materials. With respect to the latter I will also present the concept of the *Novel Materials Discovery (NOMAD) Laboratory*, a recently established European Center of Excellence: *http://NOMAD-Repository.eu*.

Cryo-EM studies of Complex Systems: Microtubule Dynamics and Transcription Initiation

Eva Nogales

UC Berkeley, HHMI, LBNL

Cryo-Electron Microscopy (cryo-EM) has emerged as an ideal technique for the structural characterization of challenging macromolecular assemblies. Recent technical breakthroughs have dramatically improved both the resolution obtainable and the capacity to describe coexisting states. We are using this methodology to gain fundamental insight into two essential and highly regulated processes in the life of the eukaryotic cell: microtubule dynamic instability and gene transcription initiation.

Dynamic instability, the stochastic switching between growth and shrinkage, is essential for microtubule function. This behavior is driven by GTP hydrolysis in the microtubule lattice, and is inhibited by anticancer agents like Taxol. We have obtained new insight into the mechanism of dynamic instability, based on high-resolution cryo-EM structures of microtubules in different nucleotide states and by characterizing the interaction of microtubules with proteins that regulate dynamic instability.

Eukaryotic transcription initiation requires the assembly of general transcription factors into a pre-initiation complex (PIC) that ensures the accurate loading of RNA polymerase II (Pol II) at the transcription start site. We have used an in vitro reconstituted system to study the assembly of human TBP, TFIIA, TFIIB, Pol II, TFIIF, TFIIE and TFIIH onto promoter DNA using cryo-EM. Our structural analysis provides pseudo-atomic models of the PIC and its engagement with DNA, before and after promoter opening.

Structural Insights into Life and Death of a Bug

Stefan Raunser

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Muscular movement plays an essential role not only in our lives. Muscle contraction is initiated by the release of calcium from the sarcoplasmic reticulum into the cytoplasm of myocytes through ryanodine receptors. Calcium binds to troponin, which releases tropomyosin from its blocking position allowing myosin filaments to move along actin filaments resulting in the contraction of the muscle. In my talk I will present our recent cryo-EM structures of the mouse ryanodine receptor 1 in its open and closed state, F-actin in complex with tropomyosin and the F-actin-myosintropomyosin complex. The structures reveal the mechanisms involved in muscle contraction at an unprecedented level of molecular detail.

Upon infection with bacterial pathogens, F-actin, which is not only the major component of muscles but also the cytoskeleton, is attacked by Tc toxin complexes. Tripartite Tc toxin complexes perforate the host membrane by forming channels that translocate toxic enzymes into the host, including humans. The underlying mechanism is complex but poorly understood. In my talk I will present the first highresolution structure of a complete 1.7 MDa Tc toxin complex composed of TcA, TcB and TcC. TcB and TcC form a large cocoon, in which the toxic domain resides and is autoproteolytically cleaved. Our results allow us for the first time to understand key steps of infections involving Tc toxins at molecular level and shed new light on the interaction of bacterial pathogens, such as the plague pathogen *Yersinia pestis*, with their hosts.

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From STED Microscopy to STED Lithography

Thomas Klar

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In 1873, Ernst Abbe has found that resolution in microscopy should be limited to a third of the wavelength.[1] This so called diffraction limit kept its dogmatic character for about 130 years, which is surprising because modern quantum chemistry and quantum optics, which were fully developed at the end of the twenties of the last century, provide basically all necessary ingredients to break this limit. Nevertheless, this fact was ignored for about 65 years until Stefan Hell dared to tackle this dogma and to postulate that taking quantum physics and –optics seriously could possibly break the Abbe diffraction limit.[2]

This talk will briefly sketch the experimental realisation of a STED microscope [3] and related techniques. On top of imaging, STED can also be used to improve the resolution and decrease the structure size in lithography, which was postulated in the early days of STED [3] but realized only recently[4,5]. This enables writing three dimensional structures comprising sizes of some tens of nanometers only. The structures show good biocompatibility and allow for bio-functionalization with proteins, down to the single protein level [6,7].

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Principles of biomolecular design

Ebbe Sloth Andersen

Interdisciplinary Nanoscience Center, Aarhus University, Denmark

A major goal of nanotechnology is to be able to rationally design and assemble advanced shapes and devices at the nanoscale. One approach to achieve this goal is to "learn from nature" and use biomolecules as a programmable and self-assembling building material. The rational design of biomolecular structure requires a detailed understanding of how the residue sequence of a biopolymer defines the self-assembly of its final three-dimensional structure. Despite the difficulty of this "folding problem" scientists have had initial successes in rationally designing and folding complicated molecular shapes using both DNA, RNA and protein [1,2,3]. In this talk I will review the current progress in biomolecular nanotechnology and describe the current design principles that allow for the successful creation of well-defined biomolecular shapes and devices. With examples from my own research on designing RNA nanostructures [2] I will focus on the considerations of geometry, topology and kinetics that are required for designing RNA structures that fold during synthesis. In this context I will introduce graph theoretical approaches for biomolecular folding, a geometry-topology analysis method that allows mapping of the folding process, and sequence design methods that might allow larger RNA nanostructures to be realized. At last I will discuss how the employed theoretical-experimental design cycle will allow us to investigate and understand the folding process in more detail.

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Improving Material Simulations with the Dynamical Mean-Field Theory

Ulrich Schollwöck

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In the last 25 years, dynamical mean-field theory (DMFT) has developed into one of the most important numerical methods for the simulation of strongly correlated quantum systems. Starting out from model Hamiltonians, the method is now becoming important for real materials where density functional theory is not sufficient due to strong correlations (i.e. no good exchange functional). The bottleneck of DMFT is the development of so-called impurity solvers, which limits the degree of realism of the simulations. The current method of choice is continuous-time quantum Monte Carlo, which however faces strong methodological limitations. In this talk, I will show how new impurity solvers based on matrix-product states (MPS/DMRG) will allow us to circumvent these limitations, making new material classes accessible.

Simulating Organic and Hybrid Electronic Devices

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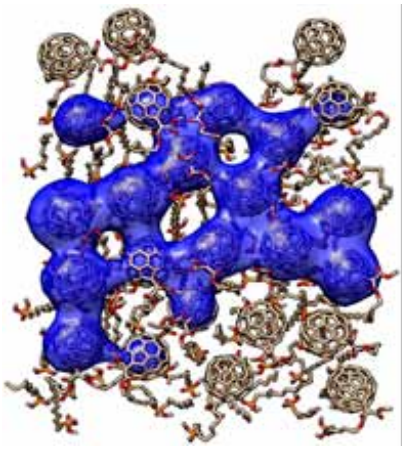
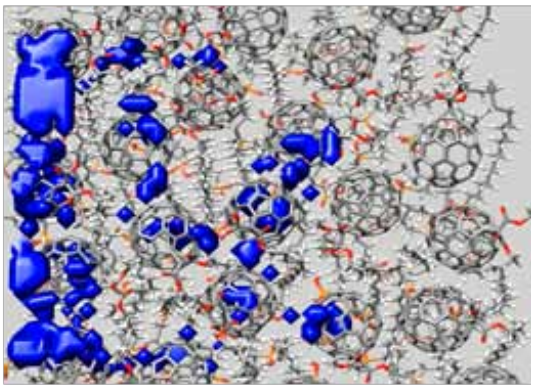
Advances in computer hard- and software are now making it possible to treat complete nanoscale devices with semiempirical molecular orbital (MO) theory.[1,2] This opens the possibility of simulating charge transport through crystals,[3] in self-assembled monolayers (SAMs)[4] or across domain boundaries by using the local ionization energy[5] or the local electron affinity,[6,7] as the external potential in specific simulations of the quantum movement of the holes or electrons, respectively. We have implemented two different techniques; explicit electron/hole dynamics on single charges and diffusion quantum Monte-Carlo (DQMC) simulations[8] on more realistic systems with many charges. The former provide us with a time scale for the charge mobility that enables us to judge mobilities in the latter simulations, which do not have an explicit time axis. The charge-transport paths obtained with these techniques agree with each other and with calculations based on Landauer theory using the semiempirical wavefunction.[9] Examples of mobility calculations in crystals and SAMs and of calculated current/voltage curves for SAM-based field-effect transistors will be given. The figure shows the path of an electron through a SAM-based device calculated using a diffusion-equation approach (left, total path) and from a virtual electrode using DQMC simulations (right, snapshot, electrode outlined in yellow).





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Developing Chemical Reaction Network Computers

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DNA nanotechnology has provided instantiation for many of the ideas of chemical reaction network theory, providing some credence to the notion that it might be possible to design computational devices that work off of chemical diffusivity rather than electronic coupling. However, it is still unclear how complex CRN computations or computers might be developed. We have begun to use NextGen sequencing platforms to implement dense chemical 'memories,' and have attempted to develop diffusion 'operators' based on DNA nanostructures that can move between and change the state of individual memory positions.

Molecular Tools for Advanced Single-Molecule Studies

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Specific attachment and tethering strategies are of utmost importance to study single biomolecules, e.g. in force and fluorescence spectroscopy. To this end we implement and improve molecular tools for use in e.g. AFM-based Single-Molecule Force Spectroscopy (SMFS). The biotin:(Strept)avidin interaction inevitably comes to mind, whenever detection, trapping or purification of biomolecules is desired. Derived thereof, the Strep-Tag II peptide/Strep-Tactin pair eliminates the necessity of biotin-labelling when working with protein specimens. As for (Strept)avidin, the tetravalency in Strep-Tactin is unfavourable for single-molecule applications. We therefore developed a monovalent Strep-Tactin featuring well-defined binding geometry and stoichiometry, yet unaltered affinity towards Strep-Tagged proteins. A unique Cysteine allows for selective immobilization or fluorescence labelling of this construct. We exploited the mechanical properties of the Strep-Tag II:monovalent Strep-Tactin interaction utilizing AFM-based single-molecule force spectroscopy. Rupture forces up to 200 pN are observed, which is comparable to biotin:(Strept)avidin unbinding. The applicability of the system in various force spectroscopy settings to study proteins of interest is evident. In addition, monovalent Strep-Tactin can be considered a precision tool that can replace (Strept)avidin in various applications, especially in mechanically demanding environments and when utilization of the genetically encoded Strep-Tag II is preferential to biotin-labelling. We utilize this novel tethering strategy to for example characterize force-sensing kinases, like Myosin Light Chain Kinase and Focal Adhesion Kinase in AFM SMFS experiments.

Engineered ribozymes as synthetic genetic switches

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Genetic switches that enable conditional gene expression are promising tools for biotechnology as well as future gene-therapeutic applications. We construct RNA-based switches of gene expression that mimic naturally occurring riboswitches. Our strategy is based on a very modular design utilizing catalytically active RNA motifs such as the Hammerhead and Twister ribozymes. Ligand-binding activities are introduced into the motifs which then allow the regulation via addition of small molecular triggers. A range of different RNA classes (mRNAs, tRNAs, rRNA, RNAi) in a wide spectrum of host cells can be controlled. In addition, ribozyme-based gene switches show superior performance in settings where the coding space is limited as well as when the additional expression of regulatory protein co-factors causes problems. Applications of ribozyme switches ranging from the implementation of genetic Boolean logics to controlling oncolytic viruses will be presented.

DNA Nanotube Nucleation: how it happens and what it can do for you

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DNA nanotubes are important as a structural primitive that bridges the molecular and material scales. To realize their potential in micron-scale construction will require the ability to position nanotubes relative to one another and/or other structures. A favored strategy for precision placement is to prepare a super-saturated solution of nanotube building blocks (“tiles”) and nucleate growth from pre-formed nanotube fragments, or “seeds". At present, however, the quality of super-saturation achieved with DNA tiles is marginal: under the narrow conditions that favor seeded nucleation, nanotube growth is so slow that spontaneous (unseeded) nucleation also occurs before seeded nanotubes grow to micron lengths, limiting the power of the seeded approach. Thus greater fundamental understanding of and control over DNA nanotube nucleation kinetics is needed.

In this talk I will (i) present an experimental determination of the size of the critical nucleus for spontaneous nucleation of HX-tiled DNA nanotubes with a defined number of double helices in circumference, (ii) deduce a strategy for augmenting the nucleation barrier and (iii) demonstrate the utility of controlled nucleation with a device built from DX-tiled DNA nanotubes.

Poster Abstracts - Session I (A-Ma)

Poster Abstracts - Session II (Mi-Z)

Investigation of Domain Folding in Maltose Binding Protein using three color single molecule FRET

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Most protein folding studies have been done on single domain proteins. However, genome analysis shows that more than 70% of the eukaryotic proteome consists of multi-domain proteins. Understanding the rules governing the correct folding of multi-domain proteins is therefore of high interest. Recent advances in single pair FRET studies have provided new insights into the mechanism of protein folding. We have developed a 3-color FRET technique which has the potential to observe coordinated motions in a protein in great detail, e. g. coordinated folding of two domains in a single protein. As a test system for folding of multi-domain protein, we have chosen a slow folding mutant of Maltose Binding Protein called Double Mutant- Maltose Binding Protein (DM-MBP). It has two domains, N terminal and C terminal domain. To apply 3-color FRET effectively, it is necessary to specifically label all three fluorophores. By choosing three precise labeling positions, specific labeling strategies and 3-color FRET, we are now in a position to investigate how the two domains coordinate each other during DM-MBP refolding from its denatured state. I will discuss the labeling approaches we have used and will present initial 3-color FRET results on the specifically labeled DM-MBP.

Contact-less visualization of fast charge carrier diffusion in hybrid halide perovskite thin films

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Organic-inorganic metal halide perovskite solar cells have recently attracted considerable attention with reported device efficiencies approaching those achieved in poly-crystalline silicon[1] or copper indium gallium selenide (CIGS)[2]. Key for an efficient extraction of photo-generated carriers is the combination of low non-radiative relaxation rates leading to long carrier lifetimes and rapid diffusive transport. The latter, however, is difficult to assess directly with reported values varying widely. We developed a novel approach for a contact-less visualization of the charge carrier diffusion length and velocity in thin films based on time-resolved confocal detection of photoluminescence at varying distances from the excitation position. Our measurements on chloride-treated methylammonium lead iodide thin films, the material for which the highest solar cell efficiencies have been reported, reveal a charge carrier diffusion length of 5.5 - 7.7 µm and a transport time of 100 ps for the first micrometer[3] corresponding to a diffusion constant of about 5 - 10 $cm^2 s^{-1}$, similar to GaAs thin films at room temperature[4].

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Atomic Force Microscopy-Based Single-Molecule Force Spectroscopy on Focal Adhesion Kinase

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Protein kinases play a key role in the regulation of cellular signaling pathways and especially in signal transduction. Focal adhesion kinase (FAK) is a non-receptor tyrosine kinase involved in transmembrane signaling, thereby regulating cell growth, migration, proliferation and development. FAK acts as a hub for cell-matrix adhesion signals controlling downstream proteins like Src, p130Cas, Grb2 and Graf. These pathways are supposed to be influenced by the force activation and regulation of FAK. However the activation process of FAK particularly in terms of force is still poorly understood. Until now there have been no single-molecule force spectroscopy data of FAK. An Atomic Force Microscopy (AFM) based measurement process and an analysis method to determine the characteristic unfolding pattern of FAKs FERM-Kinase substructure was established. Probing FAK in presence of its substrate Adenosine triphosphate (ATP) resulted in a conformational change leading to an altered unfolding pattern. The force distributions were analyzed in order to quantify the effect of ATP binding. The observed forces were found to be in a physiological range.

Synthesis of nanosized ruthenium-iridium mixed oxides for water splitting application

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The oxygen evolution reaction (OER) as a kinetically hindered 4-e^- process represents the limiting step in the water splitting process. The synthesis of stable and at the same time cheap high performance OER catalyst materials is an ongoing research challenge. The performance of a catalyst can be either improved by increasing the catalytic surface area by means of nanostructuring.[1] Another possibility is doping (cobalt / nickel) of a highly active OER catalyst like RuO_2 to lower the required overpotential.[2] In the current work a recently proposed synthesis approach of flash oxidation with potassium superoxide (KO_2) in aqueous solution was used to synthesize pure and cobalt containing ruthenium-iridium mixed oxides.[3] TEM and DLS measurements revealed the amorphous nature of the $RuIrO_x$ nanoparticles with sizes down to 0.6 nm and a high tendency of aggregation. Catalyst thin films on FTO were prepared by successive drop casting and followed by calcination in air. Electrochemical measurements revealed a minimum OER overpotential of as low as 210 mV for Co containing $RuIrO_x$. A mass normalized oxidation current of 1115 mA/mg at 1.8 V vs. RHE was obtained for the same catalyst film which was 28 % higher than recently published state of the art values of pure $RuIrO_x$ catalyst [1]. The beneficial effect on catalyst performance obtained by synthesis of ultra-small catalyst nanoparticle and successive low temperature calcination at 300 °C was shown in this work. A positive effect of Co doping on the catalytic activity and stability revealed the potential of this approach towards the synthesis of high performance, cheap and stable OER catalyst material.

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Silver-nanoparticle containing diamond-like carbon – an antimicrobial and wear-resistant surface modification

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Due to the demographic change, there is an increasing number of people of higher age. Hence, there is also a growing need for total joint replacements, e.g. hip- or knee prosthesis. To lower the number of revision surgeries and to reduce stress for the patients, it is of paramount importance to extend the lifetime of such implants and additionally improve wound healing properties. Our contribution to achieve these aims are hard and wear-resistant diamond-like carbon (DLC) surfaces in combination with various orthopaedic base materials. Additional biofunctionality of the surface modification is achieved by antimicrobial effective silver nanoparticles. We modify our surfaces by two different methods: In the coating method we deposit a polymer film containing silver nanoparticle on the substrate using a sol-gel process and afterwards we transform the polymer layer into DLC by plasma immersion ion implantation. Whereas the modification method consists of the implantation of silver ions in polymer substrates followed by the transformation of the polymer surface into diamond-like carbon by ion irradiation. To prove the successful DLC transformation, we measured both the typical content of sp^3-bindings of roughly 35% and the increased nanohardness up to 14 GPa. Under physiological conditions in vitro, silver ion release was determined with decay-times between 2 hours up to 6 days with a total silver ion release of 0,6µg/cm^2 up to 15,2µg/cm^2. In summary, we present hard, wear-resistant medical implant surfaces with an adjustable antimicrobial activity both with respect to time and concentration.

Using Fitness Landscapes to Explore the Sequence-Structure-Function Relationships of an Evolved Riboswitch

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Elucidating the relationships between the sequence, structure, and function of active biopolymers remains an important, yet unrealized goal across many disciplines. An ideal means to investigate such sequence-structure-function relationships entails creating fitness landscapes to describe small functional RNAs generated through *in vitro* directed evolution. We are creating a computational infrastructure to automate the creation and analysis of fitness landscapes based on both sequential and structural similarity. Our initial analyses will be performed on an evolved version of the $preQ_1$ riboswitch, for which the expression platform (EP) region has been randomized and subjected to *in vitro* selection. In general, riboswitches are *cis*-regulatory elements found in the 5'-UTR of mRNA, and are comprised of an aptamer (serving as a detector of its ligand) and an EP, which adopts one of two conformations, depending on the binding state of the aptamer. One binding state allows the expression of the mRNA, and the other prevents it; thus, a riboswitch acts as an "on/off switch" for a gene. Because the randomized EP region of the $preQ_1$ riboswitch is so short (19 nucleotides), our selection can exhaustively probe the EP sequence space (100-1000 fold coverage). After post-selection-sequencing, the functionally active sequences are counted and organized into fitness peaks based on sequence similarity. Secondary structures are then predicted for all sequences, which are subsequently re-sorted based on structural similarity. Because fitness landscapes essentially map sequences or structures to functional activity, we believe that comparing the sequence- and structure- based landscapes will yield new insights into sequence-structure-function relationships, which should allow more effective *in silico* predictions of the best sequences from directed evolution experiments (for any small functional RNAs), and minimize experimental testing and optimization.

Intracellular chromobody delivery by mesoporous silica nanoparticles for live cell imaging

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Chromobodies have recently drawn great attention as bioimaging nanotools thanks to their antibody-like properties. They have comparable antigen binding specificity and affinity to conventional antibodies, but smaller size and higher stability. The significant achievement of the chromobody development is that chromobodies can be used in live cell imaging for spatio-temporal visualization of cellular processes. Due to their small size they don't interfere with these processes. In this work, we developed multifunctional large-pore mesoporous silica nanoparticles (MSNs) as nanocarriers to directly transport chromobodies into living cells for endogenous antigen-visualization in real time. Multifunctional large-pore MSNs have high loading capacity for chromobodies (70 µg chromobody/mg MSNs) and are efficiently taken up by cells (more than 90 % of cells taken up MSNs in 2 h incubation). When chromobodies escape from the endosomes, the co-localization signal of fluorescent endogenous antigen and organic dye labelled chromobodies can be detected. Various endosomal release triggers were further examined to enhance the endosomal release of chromobodies. The results showed that short incubation with appropriate triggers results in a significant increase of chromobody release efficiency. Hence, in combining these two nanotools (chromobodies and MSNs), we established a new approach for chromobody applications in living cells.

Intake of silica nanoparticles in lipid vesicles as function of membrane state

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The plasma membrane is a barrier any object has to overcome during cellular uptake. There are several pathways for transport of nanoscaled objects from the outside to the interior of a cell. To determine the physics of endocytosis and similar uptake observe the intake of spherical silica nanoparticles (NP) into lipid vesicles as a simple model system. The goal of our research is to understand the driving forces of nanoparticle uptake in cells using a bottom up approach trying to answer the question: "What are the crucial parameters for the control of endocytosis-like uptake?". NP intake depends strongly on the interplay of adhesion between nanoparticle and lipid membrane, membrane curvature and tension. If the adhesion energy exceeds the other energy consuming contributions, NP are engulfed by the membrane and finally taken up, if the membrane neck breaks. As engulfed nanoparticles are taken up, the vesicle surface area shrinks, which allows us to determine the NP uptake rate quantitatively by fluorescence microscopy. The membrane's mechanical properties are thermodynamic quantities and depend strongly on the membrane state. Here we demonstrate a correlation of adhesion energy and ionic strength, varied by variation of the content of dissolved sodium chloride in the colloid suspension. An increase in ionic strength leads to an increase of particle intake until it reaches its maximum saturation. This holds for fluid phase vesicles made of DOPC as well as for gel phase DPPC vesicles. Further,

the intake probabilities and rates depend strongly on NP- concentration and size, which was tested between 20nm to 140nm. Ongoing experiments focus on the role of membrane phases and phase transitions in nanoparticle intake by studying phase separated lipid vesicles at different temperatures. First results indicate an optimization of particle uptake in vicinity of the lipid main phase transition.

Linker mediated controlled formation of gold nano-assemblies

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Plasmonic metal nanoparticles (NPs) display localized surface plasmon resonances (LSPRs) that can be tuned by controlling their shape and size, but also by forming nano-assemblies.[1] Ordered nano-assemblies contribute to enhanced plasmonic properties, including coupled LSPR modes, plasmonic heating and surface enhanced Raman scattering (SERS).[2] Hence, they find applications in photothermal therapy, catalysis, SERS chemical sensors, SERS bio-diagnostic agents and many more.[1] Motivated by this, here we have developed colloidal gold nano-assemblies with control over morphology, number of NPs per assembly (aggregation number) and inter-particle distance. Our strategy involves the utilization of molecular linkers in a colloidal self-assembly approach. We thus investigated the role of structurally different molecular ligands in the formation of stable colloidal gold nano-assemblies. Depending on the type of ligand employed i.e., organic molecule, linear polymer, branched polymers or DNA, we could manipulate the nano-assembly morphology and its optical and spectroscopic properties. Such customized gold nano-assemblies have potential for applications as SERS sensors.

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Biochemical circuits in cell-sized microcompartments

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In a typical eukaryotic cell, many incompatible biochemical processes are separated from each other through compartmentalization into specialized organelles. In order to mimic communication between artificial organelles, our present project aims at implementing such spatial separation within synthetic cell-scale systems using a class of biochemical reaction networks, based exclusively on in vitro transcription reactions and termed "genelet circuits".[1] Such circuits are encapsulated and studied within oil-in-water droplets surrounded by a lipid monolayer. Using a technique previously developed by the Bayley lab[2], droplets are brought into contact to form a bilayer of lipids through which small molecules can migrate from one compartment to another. Apolar species can transfer directly through the bilayer, while ions and small charged or polar molecules are transferred via transmembrane pores such as the antibiotic α-hemolysin. The genelet circuits are activated by the diffusion of chosen chemicals through this network. Unlike in bulk systems, chemical pathways can thus be separated or coupled controllably both in space and time. We will present a series of designs and implementations of spatially-resolved circuits, and experimental approaches to achieve the translocation of diverse molecules.

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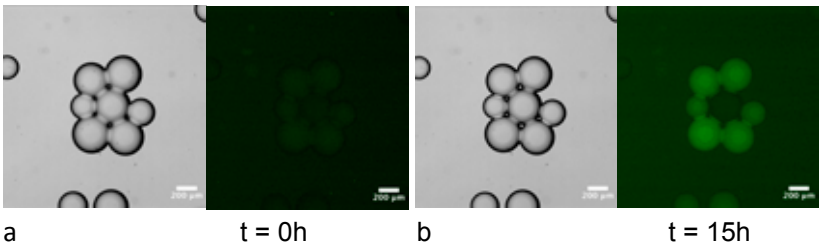

Figure 1 : Activation of a spatially-resolved circuit by the translocation a small molecule (DFHBI) through biological pores. Bright field and fluorescence images of the network at a) 0h and b) 15h after assembly.

Mapping Mechanical Force Propagation through Biomolecular Complexes

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We employed single-molecule force spectroscopy with an atomic force microscope (AFM) and steered molecular dynamics (SMD) simulations to reveal force propagation pathways through a mechanically ultrastable multidomain cellulosome protein complex. We demonstrate a new combination of network-based correlation analysis supported by AFM directional pulling experiments, which allowed us to visualize stiff and soft paths through the protein complex along which force was transmitted. The results implicate specific force-propagation architectures nonparallel to the pulling axis that are advantageous for achieving high dissociation forces.

Insight into the Photophysics of Carbon Dots

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Carbon dots (CDs) have attracted rapidly growing interest due to their exceptional advantages such as high fluorescence quantum yield, chemical stability, biocompatibility, and low toxicity.[1,2] Recently the fluorescent CDs have been used for bioimaging, photocatalysis, photovoltaics, as light-emitting diodes, and for lasing. However, due to the complex structure of CDs, the intrinsic mechanism and origin of the fluorescence in CDs have not yet been completely understood. We have recently developed a model system of polycyclic aromatic hydrocarbon (PAH) molecules embedded in a polymer matrix to reproduce the optical properties of CDs.[3] In particular, a large Stokes shift of more than 100 nm as well as excitation wavelength dependent emission properties could be achieved by fine-tuning of the concentration of only three different molecules. Therefore we conclude that Anthracene, Pyrene and Perylene molecules can be seen as the main emissive species within a CD. These results will help to enable specifically tailoring the optical properties of CDs

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Single-Molecule Organization and Detection of Enzymes

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Single Molecule Cut & Paste (SMC&P) is an AFM technique that utilizes a hierarchy of non-covalent rupture forces to spatially organize biomolecules with approximately 10nm precision. Successful transfer constructs have consisted of single-stranded DNA, DNA-RNA hybrids and DNA-conjugated proteins, such as a zinc finger motif and GFP. However, functional enzymes that are able to catalyze reactions after transport to the target surface have so far not been integrated into SMC&P. Within the current framework of the project, the system of interest would involve a catalytic reaction whose product could be detected via single-molecule fluorescence microscopy, much like previous experiments using GFP or fluorescently-labeled DNA. The first enzymes investigated were T7 RNA Polymerase and E. coli DNA Ligase. Preliminary results suggest that even though these kinds of enzymes are in principal well-suited, the system requires further adaption and optimization to make the entire SMC&P and readout processes feasible. Ongoing efforts are currently investigating T7 DNA Ligase and Pfu DNA Polymerase as promising candidates for integration into SMC&P.

Molecular configurations studied by small angle X-ray scattering

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The nanoworld is difficult to study, because normal microscopy is not able to resolve these nanostructures due to the diffraction limit. This limit can be overcome with techniques like small angle X-ray scattering (SAXS). We use SAXS to study molecular configurations for different types of soft matter materials. First, we study the structure of DNA origami and the influence of salt concentration on the structure. We can find a strong dependence on Mg concentration on the quality of the folded structure. Furthermore, we are able to do in-situ measurements and have a direct control of the structure during the folding process. Second, we can analyze the spacing of lipid phases prepared on silicon substrates with very high precision. In the lipid phases are functional molecules with an azobenzene group embedded. These molecules change from trans to cis configuration via illumination of uv light. This molecular change induces a strong change in the spacing of the lipid phase. The structural control of nanostructures is of high importance, but it is not possible for many conventional techniques, especially for organic or biological materials. SAXS offers a great possibility to investigate structures or even study their change in-situ.

Placing molecules and tuning their distances with Bohr radius resolution

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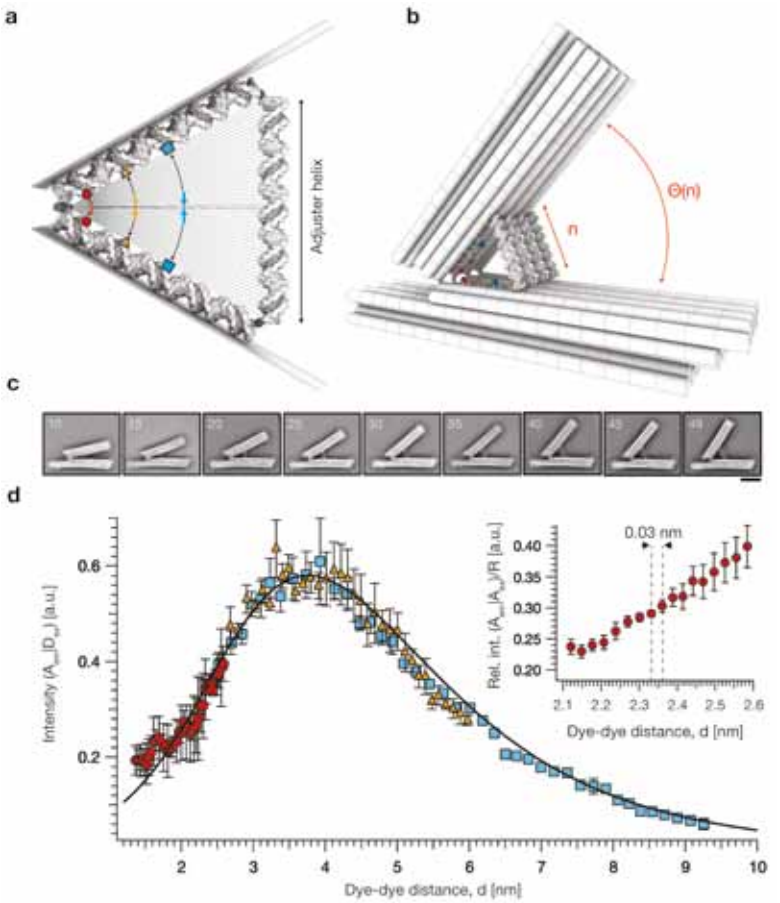
Arranging matter with ever more precision is a fundamental goal of technology. In nature, atomic scale control over molecules is achieved in proteins and enables remarkable functions, such as catalysis of chemical reactions. DNA nanotechnology is a promising candidate to match this placement accuracy seen in nature. Indeed, some objects achieve a spatial control slightly smaller than five nanometers [1-4]. Subnanometer precision however was reached only within unit cells of designed DNA crystals [5]. In this study, we rationally designed and assembled a DNA-based bimolecular positioner. To test the positioning accuracy, we used photophysical and crosslinking assays that report directly with atomic resolution on the coordinate of interest. We were able to adjust the separation of chemical moieties and fluorescent molecules from 1.5 to 9 nm in 123 discrete steps (where the smallest increment was only 0.04 nm) with fluctuation amplitudes of ± 0.5 nm.



a) Three double-stranded DNA helices that are connected through single-strand backbone bonds form the fundamental positioning unit. The number of basepairs n in the adjuster helix controls the vertex angle Θ(n). Circles, triangles, and squares indicate mounting locations 5, 15, and 25 basepairs away from hinge. **b)** Schematic illustration of the positioner apparatus. The fundamental positioning unit is embedded within the structure. Cylinders represent a double-stranded DNA segment of 10.5 basepair length. **c)** Representative 2D reference-free average micrographs of positioner variants as seen in negative-staining TEM. Numbers indicate the length of three parallel adjuster helices in basepairs in each variant. Scale bar is 20 nm. **d)** Acceptor emission intensity upon excitation of the donor dye plotted versus the dye-dye distance calculated using a geometrical model. Markers indicate mounting locations of a FRET pair according to a). Solid line: global fit to the data using a model that combines contact quenching and FRET as a function of distance. Inset: Fluorescence intensity of two ATTO 647N dyes mounted 5 basepairs away from hinge as function of inter-dye distance.

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Mesoporous Silica Nanoparticles as Platform for Targeted Drug Delivery

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In recent years colloidal mesoporous silica core-shell nanoparticles (MSN) have attracted great attention as versatile vehicles for targeted drug delivery. They possess a high pore volume, defined and tunable pore sizes and various functionalization possibilities of the inner and outer surface.[1] This allows for surface coating and/or the attachment of suitable molecules to achieve stimuli responsive pore sealing and opening. If there are altered levels of disease-specific enzymes, stimuli-responsive drug release from MSNs can be achieved by attaching a short biotinylated, enzyme-responsive peptide linker in between the MSNs and the capping system.[2] Hereby a protein can be employed as a plug, e.g. avidin which shows a very high binding affinity towards biotin.[3] Here, we report the synthesis of mesoporous silica nanoparticles containing enzyme cleavable peptide linkers attached via biotin to avidin caps. The successful uptake of MSNs and the intracellular release of the encapsulated guests is monitored by confocal microscopy.

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Direct Selection of RNA aptamers for fluorescence enhancement

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**MG and GS contributed equally to this work*

To improve *in vitro* methods for evolving RNA aptamers, we develop monoclonal **G**ene-linked **R**NA **A**ptamer **P**articles **(GRAPs)**. We applied this method to screen libraries for RNA sequences that demonstrate fluorescence-enhancement upon binding the non-fluorescent dye, Malachite Green. Our approach is the first *in vitro* selection-for-function scheme that allows direct quantitative fluorescence measurement of individual sequences followed by sequence partitioning in a high-throughput format. We select RNA aptamers that enhance the fluorescence quantum yield of Malachite Green over 1000-fold with binding on par with existing aptamers. The capability to discriminate discrete spectral profiles produces a consensus hairpin with a unique blue-shifted fluorescence maximum never before observed. We further our findings by generating libraries biased with the relevant consensus motifs to demonstrate greater improvements to fluorescence enhancement. Ultimately, this method could be used to select for RNA aptamers that exhibit any arbitrary function.

Setting up an Optical Tweezers Transducer for Determining the Mechanical Properties of Myosin

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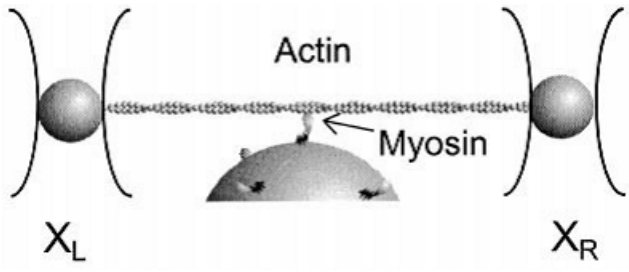
Myosins form a large family of actin-based motor proteins that are involved in different forms of cellular motility. Those include muscle contraction, intracellular transport, endo- and exocytosis, cell division and locomotion. The force and movement is produced by a change in conformation of the bound actomyosin complex (or "cross-bridge"). This process is known as the "working stroke". Here we introduce a setup for single molecule measurements. We measure the stiffness and working stroke of a single cross-bridge of Myosin with an optical tweezers transducer. The measurements are made with the "three bead" geometry devised by Finer *et al.* (1994). By this setup two beads, supported in independent optical traps, are used to hold an actin filament in the vicinity of a myosin molecule, which is immobilized on the surface of a third bead as shown in the cartoon. The movements and forces produced by actomyosin interactions are observed by detecting the position of both trapped beads with a four-quadrant-photodiode.



The "three-bead geometry" is used to make single-molecule mechanical measurements from actomyosin. Two latex beads holding an actin filament are manipulated in two independent optical traps. This filament is in the vicinity of a third bead that is coated with myosin. Actomyosin interactions are monitored by measuring the position of the trapped beads with a photodetector (giving the bead positions, XL and XR). Adapted from Veigel et al. (1998)

Single molecule imaging in living *Drosophila* embryos with reflected light-sheet microscopy

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Searching the field of light microscopy techniques for single molecule imaging *in vivo* suggests total internal reflection microscopy (TIRFM) as one of its most prominent members. However, TIRF has the major limitation that it is constrained to the imaging depth of several hundred nanometers close to the coverslip surface. The need for alternative imaging techniques is therefore evident. In order to achieve a signal-to-noise ratio (SNR) conducive to single molecule imaging, we adapted reflected light-sheet microscopy (RLSM) as described by Gebhardt *et al*. (2013) to image *Drosophila* embryos. Alignment steps were modified by means of using commercially available micro prisms attached to standard cover slips.

In fact, we were able to image a member of the septate junction complex outlining the 3D epidermal structures of highly opaque late-stage *Drosophila* embryos. Furthermore, we show freely diffusing single 10 kDa Dextran molecules conjugated to 1-2 Alexa647 dyes inside living embryos. We demonstrate that Dextran diffuses quickly (~6.4 $\mu m^2/s$) in free space and obeys directional movement within the epidermal tissue (~0.1 $\mu m^2/s$). Our results suggest that RLSM will be helpful in studying heterogeneous trafficking of single proteins to particles in multicellular organisms.

Determination of charge carrier mobility by energy dependent time-of-flight studies in mixed halide perovskite thin films

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Hybrid perovskite materials are promising candidates for incorporation in solar cell devices as they already achieve high conversion efficiencies and can be deposited easily from solution by employing cheap and earth-abundant materials [1]. The charge carrier dynamics and transport are crucial for well performing devices; however they are not yet completely understood and are therefore currently the focus of intense research efforts [2]. Microscopic contact-less time resolved studies on charge carrier diffusion by our group recently gave new insight into the respective transport dynamics and length-scales of chloride treated mixed halide perovskite thin films upon pulsed laser excitation [3]. Here we investigate the macroscopic mobility of charge carriers in perovskite absorber layers and correlate it to the efficiency of the respective device in order to gain more detailed information about the diffusion properties in perovskite thin films. To this end we performed complementary time-of-flight studies on different perovskite thin films serving as photoactive layers in functioning solar cells devices. We focus on the influence of chloride treatment on the perovskites as well as on the effect of different cations in the metal halide perovskite with respect to the resulting charge carrier mobility. Our findings are discussed in terms of the respective device efficiencies, morphologies and optical properties to allow for the investigation of effects enhancing transport properties and with that the resulting device performance. The results of the time-of-flight studies will thus lead to a more detailed description of the charge carrier transport properties and mobilities in the investigated perovskite thin films.

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Fabrication and Validation of Flexible 3D Pillar Electrodes for Neural Electrophysiological Recording

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One in fifty people suffer from paralysis or other neurological disorders. How these diseases affect brain function at the neural network level remain unknown. Neural bioelectrical signals can help us unravel the dynamic properties of these complex neural networks. Multi-electrode arrays (MEAs) are used to record these electrophysiological signals from neurons in cultures; however, it has been shown that 2D cultures do not accurately represent the complex network dynamics of the neurons, which are organized and communicate in 3D *in vivo*. Culturing cells and measuring in 2D can influence the cells and signals in ways that are not natural and can lead to misleading information from the cell culture. To accurately understand the networks that are forming we must work towards culturing and recording in 3D. Flexible pillars made of polydimethylsiloxane (PDMS) and nickel were designed and fabricated and attached to a 120 electrode array. To test for functionality and biocompatibility of the array and pillars, rat hippocampal neurons were cultured on the array. These neurons were comparable in health to neurons grown on commercial flat electrode MEAs. The neurons could live up to 3 weeks in culture, and pillars recorded electrical signals with comparable signal to noise ratio (SNR) to both homemade and commercial flat electrodes. We also analyzed and compared the number of different waveform shapes detected both by the flat electrodes and pillar electrodes to determine how the material and shape of the pillars affect the detected signals. These results show promise for the pillars to be useful as a platform to study neurological disease and mutation in 3D cultures to provide more accurate and detailed electrophysiological information at cellular level resolution.

Nanoscale Chemical Interrogation via Tip-Enhanced Raman Spectroscopy (TERS)

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The spatial resolution of standard optical microscopy techniques is ultimately limited by the diffraction of light. For visible radiation this implies that features smaller than hundreds of nanometers in size cannot be separated. This work uses an apertureless near-field technique, referred to as tip-enhanced Raman spectroscopy (TERS), to perform optical spectroscopy on true nano-length scales. The TERS system circumvents the diffraction limit by using an atomic force microscope to control a plasmonically-active metal probe along the sample surface. This probe acts as a local optical antenna which propagates spectral information on a length scale limited only by the size of the antenna apex. Reproducible near-field enhancement of both fluorescence and Raman signals has been observed from various organic dye thin films. Additionally, the greatly increased resolution of this TERS system has been confirmed by imaging nanoscale patterns of phthalocyanine derivatives. The spatial resolution achieved in these images is estimated to be 50 nm, approximately the apex diameter of the gold probes used. This equates to surface features being observed which are 100x smaller in area than those seen by a traditional Raman microscope.

Direct observation of the first steps in gelsolin-mediated actin filament nucleation

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Actin filament elongation has been extensively studied in bulk assays. The direct observation of the nucleation process on the single molecule level, however, has not been possible due to the relatively large concentrations needed for actin filament formation. Zero-mode waveguides provide a very small observation volume, which allows the measurement of concentrations up to the micromolar range. By using zero-mode waveguides, we directly observe the binding of individual fluorescently labeled actin monomers during filament formation.

Here, we present measurements of actin filament nucleation mediated by gelsolin, a barbed-end binding protein. Our data reveal the existence of kinetic intermediates during the binding of the first two monomers to gelsolin and a concentration-dependent transition to grow beyond 5 monomers. Blocking the conformational transition associated with filament formation slows down nucleation and stops elongation. Actin filament nucleation requires flattening of the actin monomer, which facilitates association and allows further elongation.

Dynamic surface acoustic wave control of nanowire lasers

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Surface acoustic waves (SAWs) have found various applications as a radio frequency tool to probe and manipulate nanosystems. When excited on piezoelectric materials, the SAW's electric field ionizes excitons and induces spatio-temporal dynamics of the such dissociated electrons and holes. The underlying physical processes and the dynamic control of the electron-hole overlap and the resulting radiative emission has been studied on great detail in two-dimensional systems [1,2] and very recently also in one-dimensional nanowires (NWs) [3]. Such NWs have attracted widespread attention as they provide an inherently one-dimensional architecture. Using highly optically active III-V semiconductors, laser emission from single NWs was obtained up to room temperature [4,5]. Here we combine these two systems to realize a highly efficient NW laser with SAW gated repetition frequency and acoustically programmable pulse energy. Building on the two preliminary works, we performed calculations of the SAW-driven temporal carrier dynamics and the resulting dynamic modulation of the gain. We show that over a wide range of SAW frequencies ranging from 300 MHz up to 1 GHz the laser emission can be efficiently modulated by SAWs for typical 10µm long NWs. Furthermore, we demonstrate, that for two counterpropagating SAWs forming a standing wave, the switching efficiency is strongly enhanced compared to single propagating SAWs. This arises from the fact that for a standing SAW nodes are stationary and electrons and holes are shuffled back and forth in opposite directions. This gives rise to a net increase of their overlap, which in turn maximizes the gain.

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Resolving Dual Binding Modes of Cellulosome Cohesin-Dockerin Complexes using Single-Molecule Force Spectroscopy

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Receptor-ligand pairs are ordinarily thought to interact through a lock and key mechanism, where a unique molecular conformation is formed upon binding. Contrary to this paradigm, cellulosomal cohesin-dockerin (Coh-Doc) pairs are believed to interact through redundant dual binding modes consisting of two distinct conformations. Combining site-directed mutagenesis and single-molecule force spectroscopy (SMFS) we studied the unbinding of Coh:Doc complexes under force. We designed Doc mutants to knock out each binding mode, and compared their single-molecule unfolding patterns as they were dissociated from Coh using an atomic force microscope (AFM) cantilever. Although average bulk measurements were unable to resolve the differences in Doc binding modes due to the similarity of the interactions, with a single-molecule method we were able to discriminate the two modes based on distinct differences in their mechanical properties. We conclude that wild-type Doc from *Clostridium thermocellum* exocellulase Cel48S populates each binding mode with similar probability. The investigated proteins will ultimately be employed in an orchestrated assembly technique called single molecule cut and paste (SMCP). Several enzyme species are relocated on a surface in varying compositions, ratios and physical collocations to study synergistic effects in enzymatic substrate conversion. As proof of principle, multiple approaches to this goal are currently developed and tested by fluorescence readout. A microfluidic chip for *in vitro* and *in situ* fusion-protein synthesis and immobilization will be used to develop an integrated phenotyping platform to facilitate multi-enzyme assemblies and enable screening for their optimal compositions.

A novel tool to examine correlation studies of cell adhesion behavior under local shear flow

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The studies of cell adhesion behavior is crucial not only for scientific interests, but also for development of implant materials in medical engineering. Therefore, we examine adhesion phenomena of different cell-substrate combinations to thoroughly determine specific properties like adhesion strength, regarding both kinetics and magnitude. Here, we present a miniaturized (~ 100 µl) lab-on-a-chip system which allows to quantify cell de-adhesion under dynamic flow conditions of physiological relevance. Using an improved technique of shear flow measurements, so called scanning Particle Image Velocimetry (sPIV) in combination with acoustic streaming experiments on adherent cells, we are able to time resolved correlate cell de-adhesion and local shear rates, ranging from 0 - 8000 s -1, within one ensemble of identically cultured and treated cells. We combine the functionality of the software PIVDAC (Particle Image Velocimetry De-Adhesion Correlation) with a thermodynamic rate model to describe the process of adhesion and de-adhesion. In turn, ongoing studies combine these results with numerical simulations to extract cell-substrate specific properties like a dynamic adhesion strength.

Studying nucleosome interactions using a DNA-based positioning scaffold

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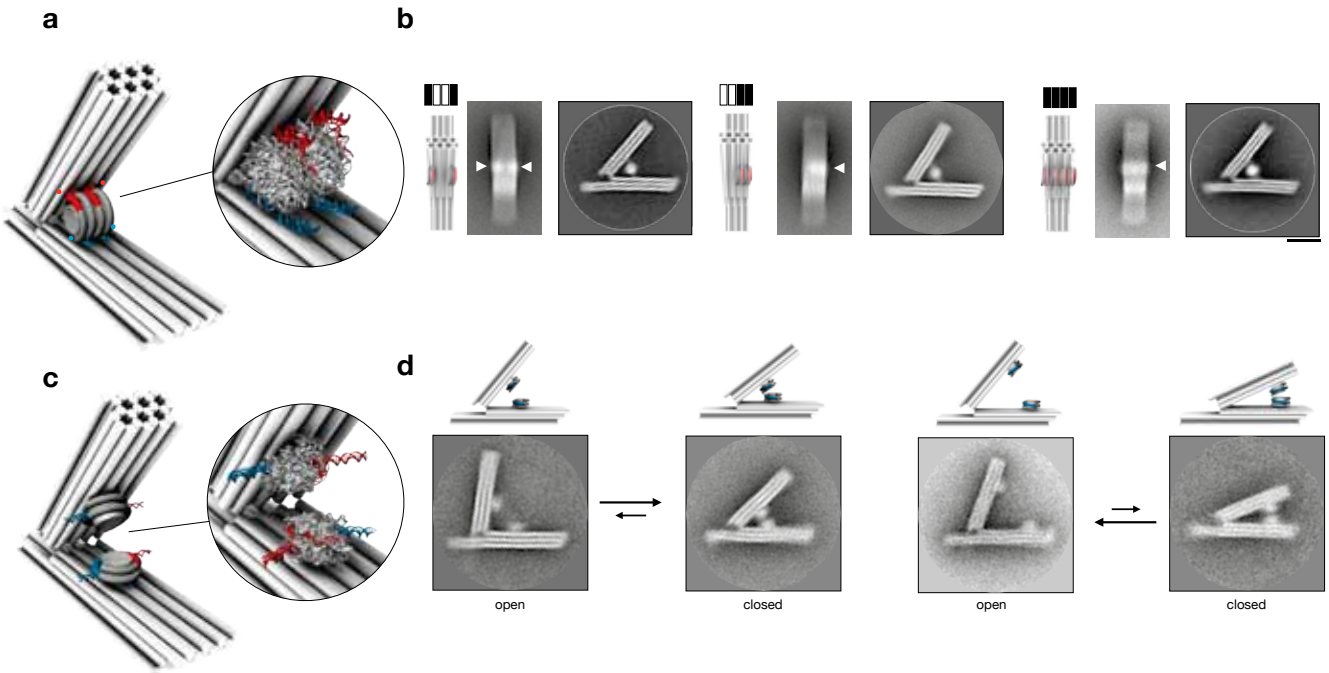
Arrays of nucleosomes structure the DNA in eukaryotic cells into chromatin fibers. The formation of these chromatin fibers is a result of complex DNA-nucleosome and nucleosome-nucleosome interactions, which are currently not completely understood. DNA nanotechnology enables the assembly of tools to precisely control matter at the nanometer scale. Using this method we rigidly positioned nucleosome core particles (NCPs) on a hinged DNA origami scaffold by means of custom designed and assembled NCPs with custom single-stranded DNA attachment handles. This enabled us to measure salt-induced unwrapping of nucleosomal DNA for a set of NCP arrangements and directly study NCP-NCP stacking as a function of NCP modifications and relative orientation. We found that the stacking interaction of two NCPs is independent of relative nucleosome orientation but strongly depends on histone tail modifications.



a) Schematic representation of the NCP-stage with two attached NCPs. Inset highlights mounting details. **b)** Average electron micrographs in top- and side view (middle, right) of three representative out of sixteen possible NCP-stage variants differing in configuration of attached NCPs. Filled squares in schematic top view (left) indicate occupied NCP mounting sites. White arrows indicate NCP positions. Scale bar is 100 nm. **c)** Schematic representation of the NCP-stage with two attached NCPs to study directly NCP-NCP stacking. **d)** Average electron micrographs of open and closed conformations, where NCPs were attached 16 nm (left) and 30 nm (right) away from the hinge.

Steps for constructing synthetic membrane curvature-inducing DNA Origami scaffolds

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Biological membranes are dynamic cellular barriers that suffer deformation and bending. Despite huge effort in identifying the general elements involved in membrane curvature, the physical-chemical basis of curvature induction is still poorly understood. In this project, we aim to fill this gap by engineering a minimal membrane curvature-inducing scaffold. Due to its exclusive nano-engineering properties, the DNA origami technology was chosen to build synthetic curvature-inducing scaffolds. This state-of-the-art technology enables the folding of long strands of DNA into nano-objects with defined shapes by using sequence-specific short DNA staples. Here, we designed DNA nanostructures with defined curvature and shape, as well as specific membrane binding positions. Hybrid origami scaffolds with specific functional membrane-attachment groups have been produced and the interaction of those hybrid scaffolds with lipid membrane model systems was studied, more precisely in terms of localization, membrane density and induction of membrane curvature. By using fluorescence microscopy, we show that the positioning and number of the membrane binding elements are essential to ensure an effective localization of the DNA nanostructures to the membrane. Moreover, the requirements seem to be dependent on the intrinsic curvature of the nanostructures. Interestingly, the quantitative characterization of our minimal membrane-scaffolds through fluorescence correlation spectroscopy (FCS) unravels that they may bind cooperatively to the membrane. In the end, our approach aims to reveal the minimal set of modules needed for shape-dependent induction of membrane curvature. In this work, we have developed and characterized the membrane binding properties of a synthetic membrane scaffold, which can act as biomimetic of the properties of biological scaffolding elements.

Plasmon Enhanced Upconversion in Single Hybrid Nanostructures Assembled by Optothermal Printing

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Colloidal nanocrystals doped with lanthanide ions can upconvert near-infrared light to visible frequencies with moderate quantum yield. One strategy to increase the efficiency is the integration with plasmonic nanoparticles, which are known to significantly increase both absorption and radiative emission of nearby luminescent materials. We show how gold nanorods can be utilized for controlled tuning of the upconverted luminescence spectrum. An all-optical approach was used to attach single hexagonal $NaYF_4:Yb^{3+},Er^{3+}$ nanocrystals at the tip of gold nanorods. Using nanorods with longitudinal surface plasmon resonances that match specific luminescence lines of the nanocrystals, we were able to tune their upconverted emission spectrum. Single-particle measurements on such hybrid structures enabled the investigation of the plasmonic enhancement effect depending on the laser polarization relative to the rod axis.

Plasmonic Focus Points for Chiral Molecule Sensing

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The chiral conformation of naturally occurring molecules plays an important role in molecular recognition processes and biochemical reactions. Chirality is also of great interest in the development of modern drugs, as it can trigger their uptake and function. Therefore, a sensitive and reliable probing of chiral characteristics is inevitable. The main part of the biomolecules absorbs in the UV-range and thus exhibits circular dichroism (CD) there. Plasmonic nanostructures can transfer the CD signal of biologically active molecules to their plasmon resonance frequency. We here present a sensor for the detection of chiral molecules built of gold nanoparticle or gold nanorod dimer with the molecule of interest located in the plasmonic hotspot. The nanoantennas are assembled on DNA origami sheets, which serve as structural element, while its B-DNA molecules are sensed at the same time. These sensors are very sensitive as they enhance the chiral signal by an order of 100 and are thus able to measure in the pM range. In addition, the signal is transferred successfully from the UV into the visible spectral region in a controlled manner. Due to the inherent addressability of DNA origami, our sensor shows great potential to place any molecule of interest in its plasmonic focus point for probing chiral properties.

Interaction of DNA origami channels with lipid membranes

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We study artificial, lipid and DNA-based systems, which mimic biological cell membranes and membrane proteins. We utilize lipid vesicles as simpler models of cells, minimizing the complexity of the systems but also retaining some of their essential features. Channel-like DNA origami structures are created and functionalized appropriately in order to mimic functions of protein channels such as membrane penetration or molecular transport. Apart from contributing to the basic understanding of channel-membrane interactions, our study may be of interest for synthetic biology applications, in which cell-like liposomes are engineered with DNA-based pores and membrane sensors. The versatility of the DNA origami technique allowed us to create a series of different pore geometries with ease. The essential feature of all three pores shown in Figure 1a is the presence of positions for hydrophobic modification. This is aimed at providing specific membrane-pore interaction, which will lead to insertion of the pore rather than just attachment to the membrane. Membrane-pore interactions are initially assessed using electron microscopy at elevated salt concentrations at which unspecific interactions are reduced. Here, we show another method of proving the presence of pores in the membrane by using a dye influx assay. These methods are complementary and together allow for a reliable statement that functionalized DNA pores are indeed inserted into the vesicle membrane. The dye influx assay involves observation of influx of external dye molecules into vesicles in the presence of origami pores. The vesicles are immobilized using biotin streptavidin chemistry, which allows observation of the vesicles for a long period. As shown in Figure 1b we see filling of the vesicles with time, whereas control vesicles without addition of the pores remain unfilled. In order to rule out simple membrane rupture and leakage, we also performed experiments with fluorophores linked to a bulky polysaccharide molecule, which is too big to enter through the pore (Figure 1c). In order to increase the concentration of DNA membrane pores, we also created vesicles encapsulating the origami structures. The effect of the pores was similar regardless of external addition or encapsulation.

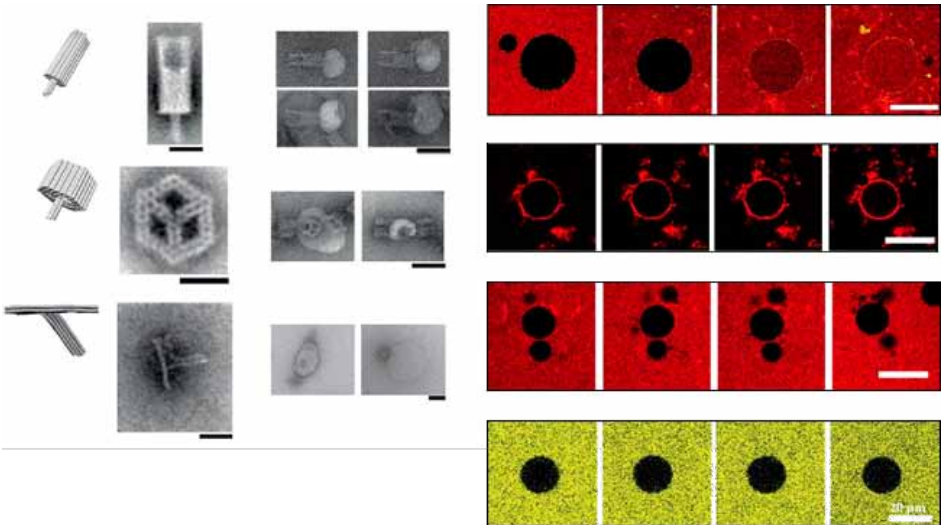

Figure1: a) Design and TEM images of the origami pores with and without lipid vesicles, scale bar 25 nm. b) Time series of dye influx in presence of pores, encapsulated pores and no pores present c) Time series recorded with a dye tethered to bulky polysaccharide, for which no influx is observed.

A synthetic codon replicator with tRNA

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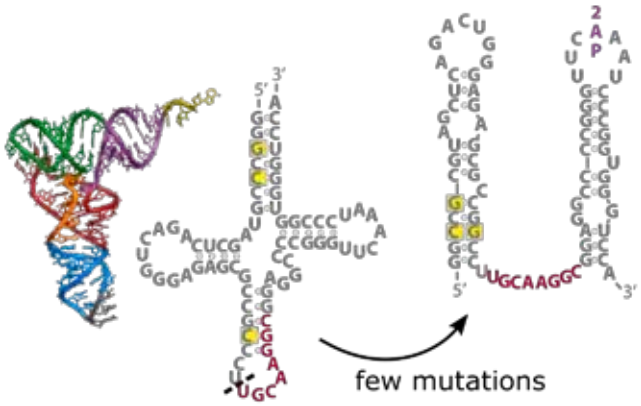
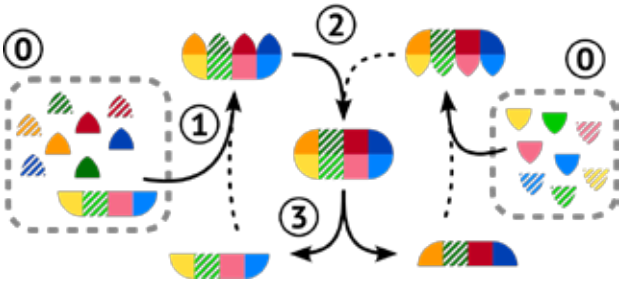
Every evolving system requires the storage and replication of genetic information. Modern biology solves this using an RNA-dominated machinery to encode proteins, which in turn replicate genetic information. However, early life most probably replicated genes using a pool of short RNA sequences. To approach the chicken and egg problem of replication using proteins, we are exploring an autonomous, waste-free, and purely thermally driven replication mechanism. Instead of error-prone chemical base-by-base replication, the mechanism operates on successions of multi-base codons. It consists of RNA molecules that encode and replicate a binary code. The RNAs are derived from transfer RNA (tRNA), each containing the anticodon framed by two hairpin loops. The anticodons serve as sequence-encoding toeholds while the hairpins are pairwise complementary, allowing the strands to bind sequentially with the anticodons aligned side by side. A central feature of the replicator is that the tRNAs' 3' ends line up upon binding, while they are close to their anticodons in the monomolecular state. The latter allows for a still-to-be-specified sequence specific aminoacylation reac-



tion. The alignment of the 3' ends permits combined interactions between the amino acids and a target, or even the formation of peptide bonds between the aligned amino acids, constituting a potential path towards protein translation. Replication of a template succession of RNAs is facilitated by temperature oscillations and proceeds in three logical steps. (1) Strands with matching anticodons bind to the template. (2) Fluctuations in the bound strands' hairpins allow for the hybridization to neighboring strands. (3) Subsequent heating splits the complementary replicate from the template, freeing both for the next cycle. In a sense, this is a physical ligation chain reaction



that proceeds cross-catalytically. Instead of chemical backbone ligation, matching strands are linked by physical base pairing.

Electrochemical Sensing of Small Molecules, Proteins, and Oligonucleotides

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The sensitive and specific detection of biological molecules of interest has applications in medicine, law enforcement, and research. However, the only currently commercially available biosensor is the blood glucose meter, the basic design and principles of which have been unchanged since its invention 50 years ago. A relatively new class of biosensors, electrochemical biosensors, generally rely on a redox-labeled oligonucleotide tethered to an electrode surface. As the electrochemically active redox tag approaches the electrode surface, the electron transfer rate between the redox tag and the electrode increases, and the transfer of electrons between the redox tag and the gold electrode is measured as current. In general, target binding changes the ease with which the redox tag approaches the surface, changing the measured current. Additionally, these systems can be "signal-on" or "signal-off", depending on the biosensor architecture used. These electrochemical sensors can be built with several different architectures: aptamer-based, (E-AB), DNA-based (E-DNA), or scaffold-based (E-Sc). Because of the variety of sensor architectures available, we can sense many classes of target, including small molecules, whole proteins, and oligonucleotides.

Towards protein-free RNA genesis

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Searching for the origin of life would be much easier, if the emergence of life started with a fully developed kangaroo hopping out of a creator's workshop. Yet, we know that life has evolved from small building blocks growing to increasingly complex and long biomolecules, towards the life we know today. One of the widely accepted hypotheses is that life started from RNA – with RNA offering both an information storage system and catalyzing reactions. But how did the first RNAzymes emerge without evolution already in place? Un-templated auto-polymerization of 3',5'-cyclic GMP is possible in dry conditions[1]. MD simulations of the base catalyzed reaction show that cGMP molecules stack onto each other[2]. However, auto-polymerization of 3',5'-cyclic nucleotides is limited to short oligomers. Is it possible to obtain RNA molecules with at least a two-base code providing an information storage capability and long enough to allow for basic catalyzing capabilities via non-enzymatic reactions? First, we confirm that – at high pH and 85 °C – base-catalyzed auto-polymerization in milli-molar solutions of cGMP can be observed. Second, we show a way to effectively ligate polyC- and polyG-oligomers with each other. This solely requires a short overhang at the 3'-end of one oligomer, and a free phosphate at the 5'-end of the other oligomer. Thus, we outline a continuous way from monomers over oligomers to long RNA molecules. Compared to 3',5'-cyclic pyrimidine-nucleotides, the stacking of 3',5'-cyclic purin-nucleotides is less stable and does not occur at temperatures above 30 °C. Thus, only the auto-polymerization of 3',5'-cyclic purin-nucleotides was reported – leading to monobasic purin-polymers that neither can store informations nor are able to grow longer by non-enzymatic ligation. Hence, we discuss ways to reduce polymerization temperature and still initiate the reaction to reach conditions where oligomeric purine could be obtained.

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[2] Untemplated Nonenzymatic Polymerization of 3',5'cGMP: A Plausible Route to 3',5'Linked Oligonucleotides in Primordia. Judit E. Šponer, Jiri Šponer, Alessandra Giorgi, Ernesto Di Mauro, Samanta Pin, and Giovanna Costanzo (2015) J. Phys. Chem. B 119,7:2979-2989.

Revealing the crystal structure of acetamidinium copper chloride

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In 1969 Bares *et al*. succeeded in synthesizing the hybrid compound acetamidinium copper chloride, $(C_2H_7N_2)_2CuCl_4$ [1]. Electron paramagnetic resonance (EPR) spectroscopy measurements pointed towards two magnetically different sites of Cu atoms. They assumed that layers of octahedrally coordinated Cu atoms are alternated with layers of tetrahedrally coordinated Cu atoms and derived a structural model from the structures of the related compounds Cs_2CuCl_4 and $(CH_3NH_3)_2CuCl_4$. However, hydrogen bonds between the Cl atoms of the predicted $CuCl_4$ tetrahedra and the amino groups of the acetamidinium cations were not taken into consideration. Since they have a crucial impact on the assembly of the organic cations and the distortion of the $CuCl_4$ tetrahedra, the model does not match the actual structure completely, which we could finally obtain from single-crystal diffraction data. The structure of acetamidinium copper chloride is discussed in detail with a special focus on the impact of hydrogen bonds.

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Site-selective ion beam synthesis of individual CdSe nanocrystal quantum dots and their coupling to silica photonic crystal nanocavities

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Ion beam implantation is a versatile tool to tailor the electronic and optical properties of semiconducting and insulating materials. In addition to doping semiconductors, fluorescing defects and nanocrystals [1,2] can be synthesized by this standard fabrication technique in semiconductor industry. Here we report on the site-selective ion beam synthesis of individual, optically active CdSe nanocrystal quantum dots (NC-QDs) using sequential ion beam implantation and their coupling to SiO_2-based nanophotonic cavities. These nanocrystals are fabricated by sequential high dose (~1at%) implantations of Se^+ and Cd^+ ions in the 200nm thick thermal oxide on a commercial Si wafer. As shown in Fig. 1, the implanted volume was confined by a structured chromium implantation mask, patterned using nanofabricated apertures with diameters ranging from 200 nm – 4500 nm. After implantation and removal of the mask, NC-QDs were formed during a rapid thermal annealing step. We demonstrate that the combination of low ion fluences and aperture diameters < 1000nm can be used to synthesize small size NC-QDs with quantum confined electronic states at low areal densities. For decreasing aperture diameter we observe a systematic blue shift of the NC-QD ensemble emission from which we deduce confinement energies exceeding 100 meV [3]. We nanofabricated one dimensional photonic crystal nanocavities [4] using large-area implanted sample material. At room temperature we achieved quality (Q) factors exceeding 10^3 over a wide energy range in the visible region. At low temperatures we demonstrate light-matter interaction in the weak coupling regime due to spectral and spatial resonance of the NC-QDs and the photonic nanocavity's mode. These light-matter coupling manifests themselves in an increase of the radiative rate and a corresponding Purcell factor FP >3 [5].

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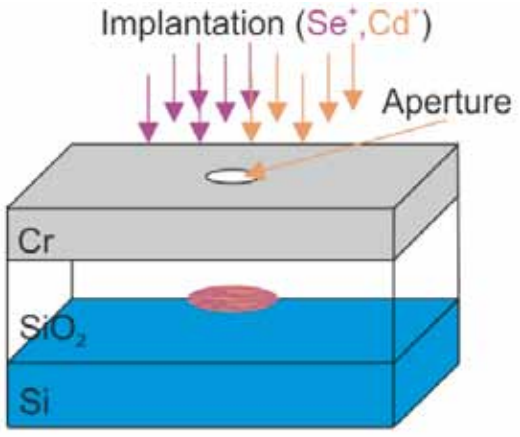

Figure 1: Schematical illustration of site-selective implantation using a chromium mask patterned with apertures.

Hole Transporter Doping for Air-Sensitive Tin-Based Perovskite Solar Cells

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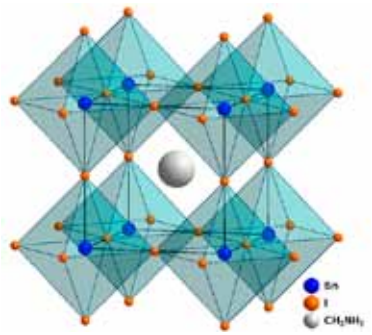

Crystal structure of the $CH_3NH_3SnI_3$.

Hybrid halide perovskites are attracting a great deal of attention in the photovoltaic field due to their demonstrated power conversion efficiencies of over 20%. However, the materials are based on a toxic element, lead, which hampers its commercial development. Alternatives in the form of tin have been proposed, but this leads to self-doping of Sn^{2+} to Sn^{4+}, resulting in oxygen-unstable devices.[1,2] This makes it unsuitable with the state-of-the-art hole transporter material (HTM) Spiro-OMeTAD, as it relies on oxygen-doping to function efficiently. In order to address this issue, here we explore alternative doping strategies. Typical solar cells rely on the oxidation of the HTM via Li TFSI in the presence of atmospheric oxygen by forming lithium oxide complexes[3] whereas protic ionic liquids such as H-TFSI promote single electron oxidation based on proton transfer from the dopant to the organic molecule operating in an inert atmosphere.[4] FK102, a Co(III) complex, is able to oxidize Spiro-OMeTAD while being reduced at the same time with an oxygen-free mechanism indicated by a direct color change.[5] A direct pre-oxidation of Spiro-OMeTAD by using Ag TFSI via a simple redox-reaction is a more controllable and reproducible way to enhance the hole-conductivity of the HTM without oxygen thus being more applicable for Sn-based perovskite solar cells.[6] In this poster we will thus compare all the different routes to doping Spiro-OMeTAD and show their effect in the prepared solar cells. Our results show that devices based on pre-oxidized Spiro-OMeTAD exhibit comparable efficiencies to standard solar cells with the prevalently used Li TFSI without exposure to air. Furthermore, the oxidized Spiro-OMeTAD with Spiro-$(TFSI)_2$ is tested as a new hole transporting system for hybrid Sn-perovskite solid-state solar cells. Thus, the results presented here allow the fabrication of $CH_3NH_3SnI_3$ solar cells without self-doping and we can therefore target higher device efficiencies.

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Selective elongation and gelation of oligonucleotides by a thermal gradient

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2 Theory of Complex Biosystems, Technical University Munich, Germany

While water, chemicals and energy are the basic ingredients for life, continuous energy fluxes are its driving forces. We could show that despite of being the lowest form of usable energy, heat flows drive a remarkable variety of origin-of-life related mechanisms inside water-filled, micrometer-sized pores. The heat flow continuously cycles the aqueous solution inside the pore via buoyancy and at the same time pushes dissolved biomolecules like oligonucleotides from hot to cold regions (thermophoresis). The two processes implement a thermal molecule trap which accumulates long (>200 bp) oligonucleotides beyond milimolar concentrations, allowing for fast intermolecular kinetics [1]. While such long strands are needed for basic replication activity [2], it is improbable that they could have formed de novo in the dilute, primordial ocean. Starting from short, sticky-ended building blocks (>18 bp) that could have polymerized by e.g. dry polymerization [3], our work shows a mutual enhancement of the concentration dependent, hybridization based strand elongation and the size-dependent accumulation of the thermal trap [4]. This results in an escalated strand elongation and, ultimately, a phase transition of the dissolved oligos into a hydrogel steady state. We propose that this dense state should simplify subsequent ligation just by keeping the strands in close proximity. Moreover, the escalated elongation and the phase transition are highly sequence selective processes because they are based upon hybridization. We could show, that only strands with self-complementary ends form a hydrogel. Strands with different self-complementary ends de-mix into spatially separated hydrogels. This mechanism could therefore sort and select for self-sticky, hence hairpin-forming sequences out of an initially random sequence pool and point towards a physical explanation for the coupled accumulation and build-up of the first structured and functional oligonucleotides.

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Photogating effect in MoS_2 mono- and few-layers

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Two-dimensional layered 'van-der Waals' materials are of increasing interest for fundamental research as well as for device applications. For optical and optoelectronic applications as well as for studying fundamental optoelectronic properties, a comprehensive knowledge about the interaction of the 2D materials with light and the dielectric environment such as the substrate is essential. We utilize inelastic light scattering for studying doping effects of mono- and few-layer MoS_2. We describe a photogating effect, which allows the control of the charge carrier density by almost two orders of magnitude without electrical contacts. Our Raman studies are consistent with physisorbed environmental molecules, which effectively deplete the intrinsically n-doped charge carrier system via charge transfer and which can be gradually removed by the exposure to light. This photogating process is reversible and precisely tunable by the light intensity. The photogating efficiency is quantified by comparison with measurements on electrostatically gated MoS_2.

We acknowledge financial support by the DFG excellence cluster "Nanosystems Initiative Munich" and Project No. Ho 3324/8-1 as well as BaCaTec.

A framework to probe receptor-ligand mechanostability

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How can we assemble protein networks? An answer to that question could have been discovered with the cellulosome, a self-assembling network of carbohydrate active enzymes, expressed by various thermo- and mesophilic bacteria, most prominently *C. thermocellum*. Assembling these enzymes into hierarchical structures, the cellulosome excels at breaking down lignocellulosic biomass. The molecular basis of this assembly process is the high affinity, high mechanostability, cohesin-dockerin receptor-ligand interaction, which we seek to understand and ultimately put to use. Using the vast set of cohesin-dockerin complexes provided by many cellulosome bearing organisms, we developed a generalized framework to compare very different receptor ligand systems mechanically using single-molecule force spectroscopy. This technique employs an AFM cantilever to measure the force necessary to sever a single protein complex or domain. By connecting receptor and ligand with a linker and stressing the complete system from N- to C-terminus using an ultrastable interaction, we are able to reversibly and reliably probe even low affinity and low force interactions. Furthermore we present initial attempts to merge these cohesin-dockerin pairs with double-stranded DNA into hybrid systems with interesting mechanical properties. The cellulosome's constituents hold the potential to become versatile couplings in nanoscopic protein assembly and have already demonstrated to be reliable tags not only for single molecule force spectroscopy experiments.

Photochemically induced electrophoresis of biomolecules for aptamer binding quantification

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The coupling of chemical reactions with physical transport phenomena can lead to intricate feedback situations. For example, ion and pH gradients across membranes are crucial for cellular metabolism and neuronal cell signaling. In this project, we optically induce localized pH gradients by photolysis of photoactive compounds, such as hexacyanoferrate or 2-nitrobenzaldehyde. Upon illumination with a focused near-UV laser, the compound releases an ion. The differential diffusion of the charged, photochemical products leads to the formation of electrical fields, as well as to pH and ionic strength gradients. As a consequence, charged molecules, such as DNA strands move characteristically within the resulting fields by means of electro- and diffusiophoresis. By choice of the photochemical compound and buffer conditions, both accumulation or depletion can be achieved. To substantiate our experimental findings we built a full kinetic model with Comsol, coupling the diffusion-migration-reaction system to the Poisson equation. As a proof of principle we were able to quantify the binding affinity of the thrombin aptamer to its target using photochemically induced electrophoresis on the microscale.

Non-equilibrium behavior of DNA hydrogels

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Comprehensive understanding of DNA hybridization thermodynamics has enabled routine construction of complex nanostructures comprised entirely of nucleic acids and governed through sequence-dependent strand interactions. With appropriate overhang sequences, these nanostructures can self-assemble into larger macrostructures, such as DNA hydrogels. Although many DNA hydrogels of sophisticated design and application have been made, relatively little is known about the non-equilibrium characteristics of DNA hydrogel structure. Here, we use a microfluidic device (i.e. a flow cell containing permeable membranes that enable buffer exchange to a sample channel) to examine the effect of salt concentration on the dynamic formation, ageing, and degradation of DNA hydrogels comprised of multivalent DNA nanostars. We observe that high salt concentrations induce hydrogel formation with two distinct phases dependent on the characteristics of the component DNA nanostars: (1) a percolated network spanning the sample channel and (2) a liquid-liquid phase separated state that localizes to the channel surface. Transitioning to low salt concentrations predictably induces degradation; unexpectedly, this process of gel dissolution exhibits structural contraction or relaxation in the system, depending on whether monovalent or divalent salt is utilized. Understanding this non-equilibrium behavior could inform future work towards constructing DNA hydrogels of increasing complexity.

DNA origami for efficient and directional energy transfer

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Understanding the interaction between light and molecules is a fundamental step towards the construction of efficient nanophotonic systems and artificial light harvesting complexes (LHC). Energy transfer phenomena typically take place at a length scale of few nanometers; therefore a precise control over the spatial arrangement of molecules is required to systematically study and manipulate light-molecule interactions. The DNA origami technique represents a versatile platform for self-assembling complex architectures made of optically active nanocomponents, such as fluorescent molecules and metal or semiconductor nanoparticles. Owing to the high specificity and programmability of DNA, precise control over the inter-molecular distances can be achieved.[1-3] In this work we use DNA origami as a platform to study energy transfer between fluorescent molecules, with a particular focus on resonance energy transfer between the fluorophores of the same type (Homo-FRET) and on how this phenomenon can enhance the light harvesting efficiency and energy transfer directionality in a system of multiple fluorophores. Inspired by nature, we also attempt to investigate the energy transfer of fluorophores arranged in a geometry resembling the antenna complexes responsible for the very efficient collection of light in natural LHCs.[4,5]

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Morphology and Performance of Organic Photovoltaics Containing a Small-molecule Acceptor

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Conjugated organic molecules are an important class of electronic materials for use in thin film electronic devices such as organic photovoltaics (OPVs). The promise of these materials is in their ability to be processed from solution enabling simple printing methods onto flexible substrates to form low cost, light weight devices. The most common type of OPV is the bulk-heterojunction (BHJ) in which the photoactive layer is comprised of a blend of an electron donating and electron accepting material to form a network structure. The photoactive layer absorbs sunlight leading to the generation of free charges that can be transported to the respective electrons. Most high efficiency OPVs use fullerene-based acceptors, but they have a high production cost, low absorption in the visible range, and limited synthetic variability of electronic and optical properties. A promising direction is new acceptor materials, which have good synthetic flexibility allowing for fine control of optoelectronic properties and may have an increased open-circuit voltage (VOC). The highest efficiencies so far for a BHJ with a non-fullerene ac-

ceptor are around 6-8% power conversion efficiency (PCE)[1,2]. Here we examine the small molecule acceptor HPI-BT [3], which was blended with P3HT to achieve a PCE of 2.1% and a VOC of 0.9V. A detailed morphological study using grazing incidence wide-angle x-ray scattering (GIWAXS), atomic force microscopy (AFM), and transmission electron microscopy (TEM) indicated that the HPI-BT acceptor crystallizes very well during film formation. However, the micron sized crystallites prevent efficient charge dissociation and thus generated charges are not being transported to the electrodes. In general small molecules crystallize very well and thus acceptor domain size needs to be reduced in order to improve device performance.

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Photocatalytic stability of single- and few-layer MoS_2

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MoS_2 is a promising two-dimensional 'van der Waals' material with outstanding electronic, optical and catalytic properties. The formation of a direct band gap in the monolayer limit, together with a high catalytic activity makes single-layer MoS_2 a very promising material for solar energy conversion by photocatalytic hydrogen evolution. We investigate the photocatalytic stability of exfoliated single- and few-layer MoS_2 immersed in an aqueous environment. The corrosion process is in-situ monitored by Raman spectroscopy. We find that while the basal plane of MoS_2 can be treated as photocatalytically stable, the edge sites and most presumably also defect sites are highly affected by a photo-induced corrosion process. Figure 1 depicts a decomposed area of a few-layer flake and the corresponding shift of the Raman A_{1g} mode after photo-corrosion in DI water. The decomposition on edge and defect sites can only be observed for excitation energies larger than the band gap energy, pointing towards the important role of photoexcited charge carriers. Furthermore, edge sites of single-layers exhibit a significantly reduced degradation under light irradiation compared to MoS_2 multi-layers. We discuss the increased stability in the single-layer case, the dependence on laser excitation power as well as excitation wavelength and the impact of oxygen present in the electrolyte [1]. We acknowledge the financial support by the DFG excellence cluster 'Nanosystems Initiative Munich' (NIM) and BaCaTec.

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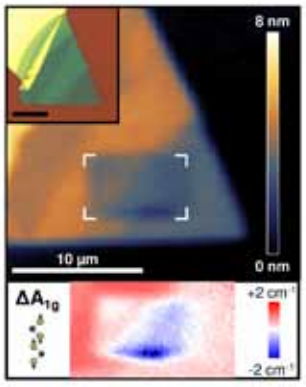

Figure: (top) White light interferometry image of few layer MoS_2 selectively decomposed by light irradiation (compare indicated area). Inset shows optical image before corrosion. (bottom) relative shift of the A_{1g} phonon mode as a function of position, demonstrating that the number of layers is reduced during the corrosion process.

Microplasma spray deposition of nanostructured $NiFe_2O_4$/NiO thin films for exchange bias applications

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Intimate contact between a ferromagnet (FM) and an antiferromagnet (AFM) can result in exchange bias (EB), a phenomenon used in magnetic sensors and data storage devices where the strong magnetic anisotropy of the AFM causes a shift in the magnetic behavior of the softer, FM material. These systems are characterized by pinning of magnetic spins at the FM/AFM interface, requiring large fields to reverse the moment of the ferromagnet. Recently, there has been considerable interest in exchange biasing magnetic nanoparticles to overcome the superparamagnetic limit (i.e., the size limit below which particle magnetization becomes unstable at room temperature), which has hampered the development of ultra high-density storage technologies. In this work, we use a novel microplasma-based spray deposition technique to realize nanostructured $NiFe_2O_4$/NiO films for exchange bias applications [Fig. 1]. Organometallic precursors are broken down in a flow-stabilized hollow cathode jet to form a directed flux of active growth species (atoms, ions, clusters, etc.), which can be spray deposited on any surface. The unique operating conditions of the microplasma, namely high $T_{electron}$ and low T_{ion}, high pressure (10 to 1000 Torr), and short space time (~µs), provide an ideal environment for cluster nucleation and growth of $NiFe_2O_4$/NiO nanogranular films. A detailed temperature and field-dependent magnetic study of these films, as well as the underlying mechanisms responsible for the EB effect will be presented.

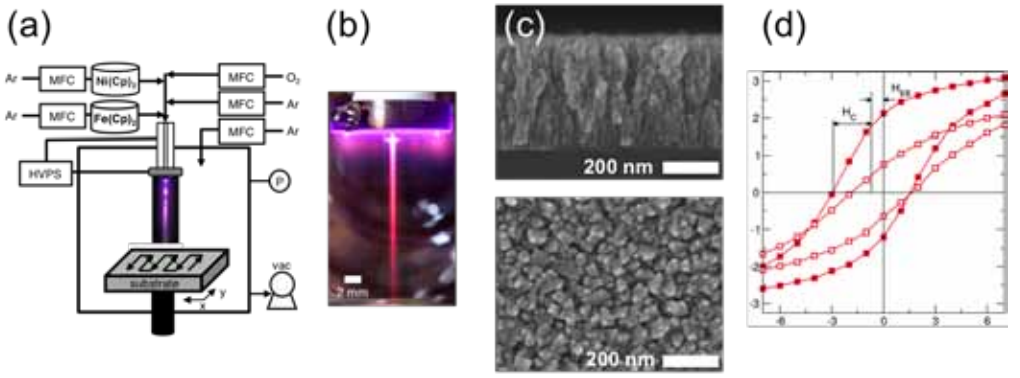

Fig. 1 (a) Schematic of the microplasma-deposition system, **(b)** picture of Argon microplasma jet operated at 14 Torr, **(c)** SEM images of cross-sectional and plan views of a $NiFe_2O_4$/NiO film deposited using microplasmas, and **(d)** magnetic hysteresis loops for a $NiFe_2O_4$/NiO film, where HC is the coercivity (half the width of the loop) and HEB is the horizontal loop shift due to exchange bias.

Extrinsic N-type Doping of Ambipolar DPP Polymers with Organometallic Dopants

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Thermoelectic materials have been of interest in scavenging waste heat; however many efficient inorganic materials are rare, brittle, and contain toxic elements. Organic thermoelectrics offer a potential alternative because they are abundant, mechanically flexible, solution processable and operative at low temperatures (<200°C). Thermoelectric devices require complementary n- and p-type legs, which ideally will have similar thermoelectric properties. A route to achieve this goal is to use an ambipolar polymer, which can be used in both legs. Here we investigate the electronic doping mechanism of an ambipolar polymer based on a co-polymer of Poly{((E)-3-(5-([8,8'-biindeno[2,1-b]thiophenylidene]-2-yl)thiophen-2-yl)-2,5-bis(2-octyldodecyl)-6-(thiophen-2-yl)pyrrolo[3,4-c]pyrrole-1,4(2H,5H)-dione} (P(BTP-DPP)) doped with organometallic small molecule dopants that lead to p- or n-type conduction. The molecular design of P(BTP-DPP) allows for efficient packing of dopants, leading to charge transfer and relatively good electrical conductivity. Transmission electron microscopy provided the dopant distribution and morphology within the doped blends. Electron paramagnetic resonance was used to determine the efficiency of the dopant in generation of charge carriers and to provide insight into the charge transport mechanism. Maximum n-type conductivities of ~10^{-1} S/cm were achieved; these values are amongst the best known for n-type semiconducting polymers.

Organometal Halide Perovskite ($CH_3NH_3PbX_3$, X = Br, I, Cl) Nanosheets with Strong Quantum Confinement

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Hybrid organometal halide perovskites ($CH_3NH_3PbX_3$, X = Br, I, Cl) have received great attention in the past few years owing to their unique properties such as high absorption cross-section, high carrier mobility and solution processability, which makes them ideal platform for high performance photovoltaic applications. The research on perovskites have been sparked by their appeal in various technological applications such as field-effect transistors, solar cells, light emitting devices and lasers, as well as for the fundamental understanding of their nanoscale behaviour. The power conversion efficiencies of over 20% has been reported by the incorporation of perovskites into solid-state solar cell devices. Although a significant amount of research has been carried out on bulk (3D) perovskites on substrates, the fundamental understanding of 2D perovskites is limited due to the problems associated with their preparation. We present a general colloidal synthesis method for the preparation of hybrid organometal halide perovskite ($CH_3NH_3PbX_3$, X = Br, I, Cl) nanoparticles (NPs) that shows strong quantum confinement and NPs that exhibit bulk like optical properties in all three types of halide perovskites. Furthermore, it was found that the NPs with bulk like optical properties generally exhibits Burstein-Moss band filling effect, whereas the confined particles with less density of energy states does not exhibit such effect. This work opens a simple synthetic route for the preparation of Perovskite NPs and offers new insights into the fundamental understanding of their nanoscopic behaviour.

On-surface synthesis of covalent organic nanostructures on metals and strategies for post synthetic decoupling

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On-surface polymerization is a versatile approach for the synthesis of otherwise inaccessible extended low-dimensional organic nanostructures. Ullmann coupling as the most favored reaction relies on the catalytic activity of metal surfaces to initiate the coupling by dissociating weakly bonded halogen substituents. Since the metal surfaces that are indispensable for the synthesis are unfavorable for many applications, we explore strategies for a post synthetic detachment. Surface chemical studies of 1,3-diiodobenzene on Cu(111) revealed covalently coupled trimers as reaction products adsorbed atop a closed iodine monolayer rather than directly on the metal surface. These unexpected results suggest iodine creeps underneath the organics, thereby indicating possibilities for using iodine monolayers for post synthetic decoupling. This approach was tested by synthesizing a covalently cross-linked 2D polyphenylene network on a metal surface and subsequently exposing the sample to iodine vapor. Samples were characterized before and after the iodine treatment by STM, XPS, and NEXAFS. Owing to the steric hindrance of σ-bonded phenyl rings the covalent network is intrinsically non-planar. However, on metal surfaces polyphenylenes become mostly planar by virtue of strong interactions. Yet, after iodine exposure the phenyl rings of the covalent network were found to be no longer parallel to the surface. In accord with STM data, these findings can be interpreted as detachment of the covalent networks from the metal surface by intercalation of an iodine monolayer. The weakened adsorption strength on the iodine monolayer allows the covalent network to adopt its intrinsically non-planar geometry.

Photoswitchable microtubule inhibitors optically control mitosis and cell death

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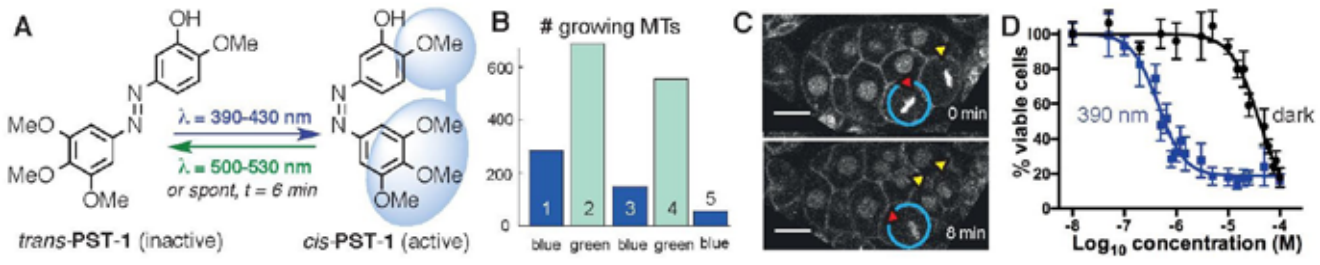
Small molecules that inhibit microtubule dynamics, such as Taxol and the Vinca alkaloids, are widely used in cell biology research and are mainstay clinical anticancer drugs. However, their activity cannot be restricted to specific cells, so they cannot spatiotemporally address the many biological processes dependent on microtubules. We developed Photostatins to overcome the nonspecificity of existing microtubule inhibitors. Photostatins (PSTs) can be photoswitched between the potent cis isomer and the inactive trans isomer, with full reversibility, using visible light (A). PSTs photoswitched in cellulo optically control microtubule dynamics with a temporal response on the scale of seconds (B). PSTs can pause or allow mitosis in living organisms with spatial precision at the single-cell level, using standard confocal microscopy (C). As antimitotics, Photostatins are >100 times more cytotoxic when switched on with blue light than when kept in the dark (D). Photostatins are powerful tools for cell biology, enabling dynamic studies of a range of microtubule-dependent processes including intracellular transport, cell motility, and proliferation. Most excitingly, Photostatins are promising as precision chemotherapeutics whose toxicity may be spatiotemporally constrained to tumours using light, for cancer chemotherapy without the therapeutically limiting, off-target toxicity of current drugs.



A: Representative compound PST-1. **B:** PSTs pause and restart MT polymerisation in living cells under alternating blue and green illumination (active MT count during timecourse). **C:** PSTs modulate embryonic development of *C. elegans* on a cell-by-cell basis: blue light pauses targeted cells in mitosis (blue ring), while neighbouring cells divide normally. **D:** PSTs are submicromolar toxins under blue light (blue curve), but >100 times less toxic in the dark (black), indicating a wide therapeutic concentration window for light-localised toxicity.

Nucleation of C70-aggregates on pentacene thin films for nanostructuring organic interfaces

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Organic heterojunctions with well defined, nanostructured interfaces are desired for the investi-gation of interface effects. We use molecular beam deposition to create model-like, nanoscale interfaces by self-assembly of C70-aggregates on pentacene thin films. Size and distribution of these fullerene-islands can be tuned by the choice of evaporation rate and sample temperature. An accompanying growth study utilizing x-ray Bragg scattering in reflection geometry, grazing incidence diffraction and atomic force microscopy on pentacene-C70 bilayer systems gives insight into the basic growth mechanism of the fullerene. In combination with in-situ measurements of thin film transistor characteristics during growth of the active layer, this allows us to correlate electronic effects, such as charging phenomena at the interface [1], with nanomorphology. In future measurements we plan to apply photoresponse microscopy [2] to study charge transfer at the pentacene-C70 heterojunction. The experiments will be complemented with an additional investigation by scanning near-field optical microscopy [3].

[1] S. J. Noever, S. Fischer, B. Nickel, Adv. Mater. 2013, 25, 2147–2151.

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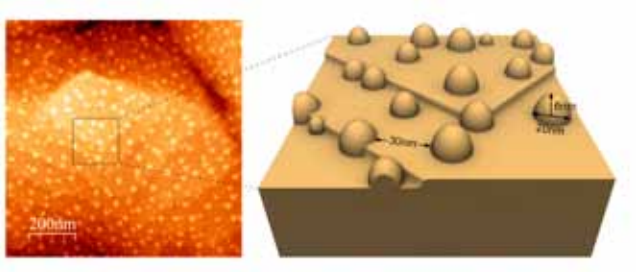
[3] C. Westermeier, A. Cernescu, S. Amarie, C. Liewald, F. Keilmann, B. Nickel, Nat Commun. 2014, 5, 4101.



DNA-PAINT and its biological application

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Since the Nobel Prize in 2014, super-resolution microscopy is in high demand, but obtaining multiplexed images for a large number of distinct target species remains challenging. A solution to this problem is DNA-PAINT, a technique which uses the transient binding of short fluorescently labeled oligonucleotides for simple and easy-to-implement multiplexed super-resolution imaging that achieves sub-10-nm spatial resolution in vitro on synthetic DNA structures. The same principle can be applied when addressing biological questions, however, what use is a sub-10-nm resolution if the labeling agents, e.g. antibodies are larger than 15 nm? To this extent aptamers offer themselves as a perfect labeling candidate. Aptamers are RNA or ssDNA strands, which fold into a three-dimensional structure when associating with their ligands and can be equal to antibodies in terms of targeting specificity and affinity. In the following, we are discussing, Aptamer-PAINT and its possibilities to overcome the current labeling difficulties.

Cell-free production and assembly of a multifunctional RNA-protein hybrid structure

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** These authors contributed equally to this work*

In order to study the dynamics of the self-assembly of a RNA-protein hybrid structure in a cell-free transcription-translation system, we encoded an RNA nanostructure with peptide binding aptamers and two proteins into a plasmid. The RNA structure (Fig. 1a) is comprised of a three-way junction with three differently functionalized arms so that each report a different step in the structure's self-organization process. The first arm reports the concentration of correctly folded RNA-scaffold. The second arm directs the assembly of a fluorescent protein-based FRET pair. The third subunit localizes the assembled nanostructure at streptavidin-coated surfaces. In a second design of the RNA structure (Fig. 1b), two arms of the three-way junction are used to polymerize the RNA molecules through kissing-loop interactions, while the third arm remains as one of the previously functionalized subunits. This will result in RNA clusters with higher local concentrations of functionalized RNA. Our work demonstrates the use of a cell-free gene expression system for prototyping and optimizing the assembly of biomolecular hybrid structures.

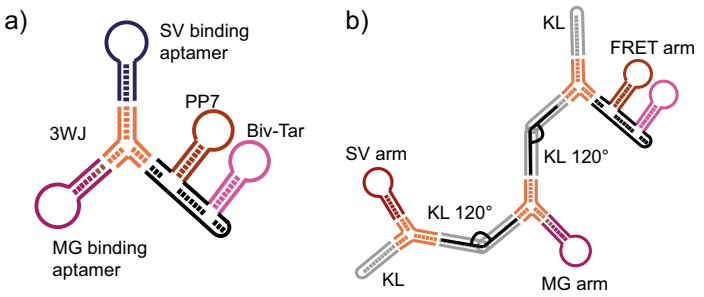

Figure 1. a) A sketch of the RNA structure with the central three-way-junction (3WJ), a Malachite Green (MG) binding RNA aptamer, a Streptavidin (SV) biding RNA aptamer, a PP7 bindings RNA aptamer for the fusion protein CFP-PP7 and a Biv-Tat binding RNA aptamer for the fusion protein YFP-Biv-Tat. **b)** A sketch of the second design of the RNA structure. Three RNA molecules are polymerized through kissing-loop (KL) interactions.

Optoelectronics of topologically insulating nanowires

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In recent years, a class of solid-state materials, called three-dimensional topological insulators, has emerged. In the bulk, a topological insulator behaves like an ordinary insulator with a band gap. At the surface, conducting gapless states exist showing remarkable properties such as helical Dirac dispersion and suppression of backscattering of spinpolarized charge carriers [1]. The characterization and control of the surface states via transport experiments is often hindered by residual bulk contributions. We utilize an on-chip photocurrent pump-probe spectroscopy based on coplanar striplines [2], to identify photocurrent mechanisms in topologically insulating Bi_2Te_2Se nanowires in the time-domain. A bias dependent photoresponse in the 100 ps regime can be interpreted to originate from photodoping due to the excitation of bulk charge carriers which relax via surface bands. We further observe a very strong polarization control of the time-integrated photocurrent response in thin Bi_2Te_2Se nanowires. The results are relevant for nanowire-based optoelectronic applications.

[1] C. Kastl, P. Seifert et al, 2D Materials 2, 024012 (2015).

[2] C. Kastl et al. Nature Communications 6, 6617 (2015).

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Size and Functionality Control of Covalent Organic Frameworks by a Modulating System

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Covalent organic frameworks (COFs) represent a unique class of crystalline materials with high potential for diverse applications.[1] By combining two building blocks via covalent bonds, 2- or 3-dimensional covalent frameworks are attainable. Due to their outstanding properties related to defined pore size, high specific surface area and structural diversity, these materials can be used in host-guest studies for gas storage, separation and catalysis. The crystalline structure implies a high degree of control of defined pore and wall topologies, pore sizes and shapes as well as a precise arrangement of active sites within the network. Recently, new steps have been taken to use COFs in organic electronics by incorporating photoactive building blocks into the frameworks.[2] Our studies on the well-known structure of COF-5 show that the crystallinity can be substantially enhanced by the addition of a reactive modulator. In contrast to the prevailing synthesis, COF-5 frameworks with extremely large domains of highly porous and crystalline structures were generated.

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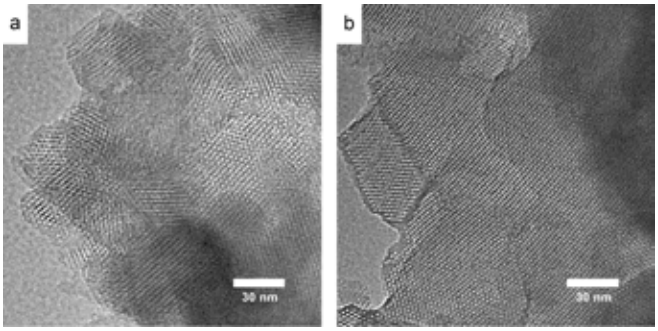
[2] D. Medina, V. Werner, F. Auras, R. Tautz, M. Dogru, J. Schuster, S. Linke, M. Döblinger, J. Feldmann, P. Knochel and T. Bein, ACS Nano, 2014, 8, 4042-4052.



Transmission electron micrographs of a) COF-5 and b) COF-5-x, synthesized in the presence of a modulating agent x.

Thermo-osmotic and Thermo-electric Effects on an Optically Trapped Janus Particle

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The optical excitation of surface plasmons in metallic nanostructures leads to strongly enhanced light scattering and absorption. During the last decade, the enhanced light absorption of metallic nanoparticles has been exploited to efficiently and controllably heat at the nanoscale.[1] However, the possibility of converting heat into mechanical motion has emerged only recently. One example from our group has been the elevation of a gold-silica Janus particle along a laser beam axis in an optical trap.[2] The propulsion mechanism is based on the local temperature gradient created around the particle itself due to the laser induced heating of the gold-coated hemisphere. Envisioning possible bio-applications for this controlled thermophoretic motion leads us to the question of whether changes in the surface charge density of the particle or in the salinity of the medium will influence their microelevation capability. To this end, we analyze the dependency of the self-thermophoretically driven motion of the optically trapped Au-silica Janus particle on the salinity and on the nature of the added electrolyte. Our experimental results witness the interplay between the self-induced thermophoretic motion of an asymmetrical particle and the solvent-particle interfacial interactions at the single particle level. Specifically, the microelevation capability of the laser-trapped gold-silica Janus particle is hindered by increasing the salinity of the medium (thermoosmotic effect). Also, the thermoelectricity of the chosen electrolytes play a dominant role on the elevation of the particle.

[1] G. Baffou, and R. Quidant, "Thermo-plasmonics: using metallic nanostructures as nano-sources of heat," Laser Photon. Rev. 7, 171–187 (2013).

[2] S. Nedev, et al, "An Optically Controlled Microscale Elevator Using Plasmonic Janus Particles," ACS photonics 2, 491–496 (2015).

Schematic representation of the axial displacement of an optically trapped Au-silica Janus particle in an electrolyte solution.

DMFT+NRG study of spin-orbital separation in a three-band Hund metal

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We show that the numerical renormalization group (NRG) is a viable multi-band impurity solver for Dynamical Mean Field Theory (DMFT), offering unprecedented real-frequency spectral resolution at arbitrarily low energies and temperatures. We use it to obtain a numerically exact DMFT solution to the Hund's metal problem for a three-band model on a Bethe lattice at $1/3$ filling. The ground state is a Fermi liquid. The one-particle spectral function undergoes a coherence-incoherence crossover with increasing temperature, with spectral weight being transfered from low to high energies. Further, it exhibits a strong particle-hole asymmetry. In the incoherent regime the self-energy displays approximate power-law behavior for positive frequencies only. The spin and orbital spectral functions show ``spin-orbital separation'': spin screening occurs at much lower energies than orbital screening. The renormalization group flows clearly reveal the relevant physics at all energy scales.

Cell guidance and electrostatic separation employing ferroelectric lithography and hydrophobic/ hydrophilic structured substrates

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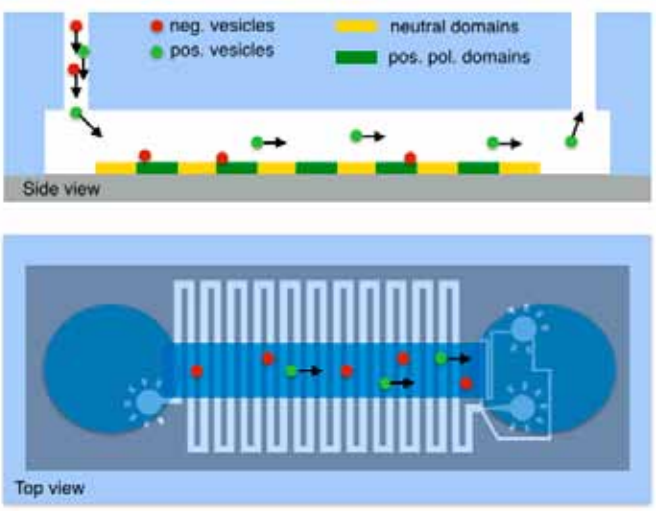
Tissue engineering and nerve cord repair has become an essential topic in biophysical and medical research. Both issues rely on the understanding of the principles of tissue growth to produce functional replacement tissue for clinical use. Therefore it is important to examine cell proliferation and migration to learn about regeneration and reassembling of tissue layer after injury or bone damage. In [1], we recently studied how surface acoustic waves on $LiNbO_3$ can be used to enhance and/ or direct cell growth. Going one step further, we now try to guide those cells along certain tracks by functionalizing the substrate surfaces in terms of their electrostatic and hydrophobic/hydrophilic properties. Due to their known hydrophilic and electrostatic interaction response, it seems very likely that cells and cell growth are sensitive to such functional domains. Being a ferroelectric material, $LiNbO_3$ can be electrically polarised (poled) by applying an external electric field along its Z-axis to obtain positive and negative domains being separated by domain walls. Such domains and domain boundaries can then be visualized by, e.g., the deposition of micro sized metal structures. To mimick cell-domain interactions, we first examine the influence of polarized domains on positively and negatively charged vesicles, as a model for electrostatically charged cell membranes. Employing a microfluidic channel system with a well defined flow profile on substrates with alternating ferroelectric domains, we determine the binding strength of red blood cells and lipid vesicles of different charge. However, not only electrostatic fields can be used to guide cells along a certain track, we also fabricated hydrophilic trails on hydrophobic surfaces to lead cell migration into desired shape. In turn, ongoing studies combine those methods to study and control cell migration and proliferation and even cellcell-interaction.



[1] M. Stamp, M. Brugger, A. Wixforth, and C. Westerhausen, "Manipulation of cell proliferation and migration using surface acoustic waves," in preparation

Photocatalytic water splitting with co-catalyst decorated CdS nanorods

Jacek K. Stolarczyk[1,2], Thomas Simon[1,2], Christian Wolff[1,2], Michael Carlson[1,2], Panajotis Livadas[1,2], Pete Frischmann[3,4], Marcus Schulze[3], Frank Würthner[3], Jochen Feldmann[1]

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Colloidal semiconductor nanoparticles hold great promise for efficient solar fuel generation. However, many of these systems suffer from low efficiencies, often determined by slow hole transfer processes. Furthermore, a failure to quickly remove the hole often leads to photooxidation, especially with Cd chalcogenides. This happens even in presence of a sacrificial electron donor. Despite the progress in the field, many open questions remain regarding the charge transfer dynamics, recombination pathways, interfacial kinetics and chemical reactions of the fuel generation reactions. Here, we present a highly efficient system which achieves over 50% external and over 70% internal quantum yield of H_2 generation using CdS nanorods decorated with nickel co-catalysts.[1] The process relies on redox shuttle mechanism in which a mediator molecule relays the photoexcited hole from the surface to the hole scavenger present in solution. The fast transfer of the holes limits the electron-hole recombination rate and – additionally - confers long-term stability on the photocatalyst. For CdS nanorods decorated with both reduction (Pt nanoparticle) and oxidation catalyst (Ru-based complex) we demonstrate that it is also possible to efficiently transfer the electron and the hole to the reduction and oxidation catalysts, respectively. This allows for the simultaneous generation of hydrogen and oxygen without the use of any sacrificial agents.[2] This way a full water splitting process is achieved. Alternatively, instead of oxygen production, oxidative dye degradation is also possible, shown for methylene blue dye.

[1] T. Simon et al., Nat. Mater. 2014, 13, 1013

[2] C.Wolff et al, to be submitted.

Single molecule force spectroscopy reveals interaction strength between *Streptococcus pneumoniae* TIGR4 pilus-1 tip protein RrgA and human fibronectin

Tanja Becke[1,2], Stefan Ness[2], Raimund Gürster[2], Arndt F. Schilling[1,4], Anne Marie di Guilmi[3], Hauke Clausen-Schaumann[1], Stefanie Sudhop[1], and Markus Hilleringmann[2]

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Gram-positive *Streptococcus pneumoniae* represents a major human pathogen causing serious diseases including pneumonia, meningitis and febrile bacteremia with high mortality rates worldwide. Among other virulence factors, recently discovered surface appendages (pili) are involved in pneumococcal host colonization and invasion. Native *Streptococcus pneumoniae* TIGR4 pilus-1 is composed of an RrgC cell wall anchor protein, multiple covalently linked RrgB backbone subunits and a terminal RrgA adhesion molecule. The pilus tip protein RrgA was found to interact with specific host components like extracellular matrix molecules (ECMs) and elements of the innate immune system. However the precise role of RrgA and the fundamental molecular mechanisms of respective individual RrgA domains during host factor interplay are not understood in detail. In particular, nothing is known about the specific thermodynamics and underlying interaction forces between RrgA mediated associations and potential consequences regarding their respective role during pneumococcal infection. In this study, we use single molecule force spectroscopy, a widely used operating mode of the atomic force microscope to directly probe protein-protein-linking, to quantify the interaction forces between the pilus subunits and different ECMs. In a first attempt we could show specific binding forces between the tip protein RrgA and human fibronectin, whereas the pilus backbone protein RrgB shows no specific binding towards the respective molecule. We plan further experiments studying thermodynamics of the RrgA – fibronectin association process applying isothermal titration calorimetry. We anticipate these studies to be a starting point for the detailed analysis of the molecular interplay between the pneumococcal type-1 pilus subunits and various host ECMs like fibronectin, laminin, collagen I as well as elements of the host innate immune system and potentially whole cells.

Quantum confinement in diluted organo-metal halide perovskite suspension with ligand

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$CH_3NH_3PbBr_3$ perovskite nanoparticles are synthesized using octylamine as ligand to avoid the formation of huge crystals. By increasing the amount of ligand, the perovskite suspension exhibit an obvious blue shift, which is probably due to the effects of quantum confinement in the $CH_3NH_3PbBr_3$ perovskite thin sheets as previously reported. The blue shifted emission also shows a shortened lifetime compared with the common $CH_3NH_3PbBr_3$ perovskite luminescence at around 520nm. Interestingly, with the dilution of perovskite suspension using toluene as solvent, the fluorescence color changes from green to bluish green and then to pure blue under UV light. Photoluminescence spectra shows that emission components at shorter wavelength emerges in diluted perovskite suspension and corresponding absorption peak can be found in the absorption spectra. The diluted perovskite suspensions with blue shifted emission shows an increased lifetime compared with the non-diluted ones. In all cases, the result of size distribution analysis shows that the suspension contains particles with the size of 100nm-500nm, in consistent with TEM images, which represents the perovskite platelet with different thickness. A surprisingly significant blue shift caused by quantum confinement is also observed in $CH_3NH_3PbI_3$ perovskite suspension. While the suspension is diluted with chloroform by 10 times, the emission shifts from 760nm as normal to bright orange color centered around 550nm, corresponding well to the luminescent behavior of bi-layered $CH_3NH_3PbI_3$ perovskite 2D platelets.

Decomposition of single retroviral integration events: intermediates and transition kinetics

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Retroviruses, such as the human immunodeficiency virus (HIV), require to covalently insert a double-stranded DNA copy of their genome into the chromatin of the host. This process is referred to as integration, and represents a point of no return in the infection cycle. In order to find improved strategies for the eradication of HIV, a better understanding of the integration process is required. We are currently investigating retroviral integration at the most fundamental level - the level of single molecules - in order to provide unprecedented information on structure-function relations and transition kinetics throughout individual cycles of HIV integration catalysis. To this end, we use a combination of atomic force microscopy (AFM) imaging and magnetic tweezers. In this contribution we present our research strategy and summarize our latest findings.

From Genes to Protein Mechanics on a Chip

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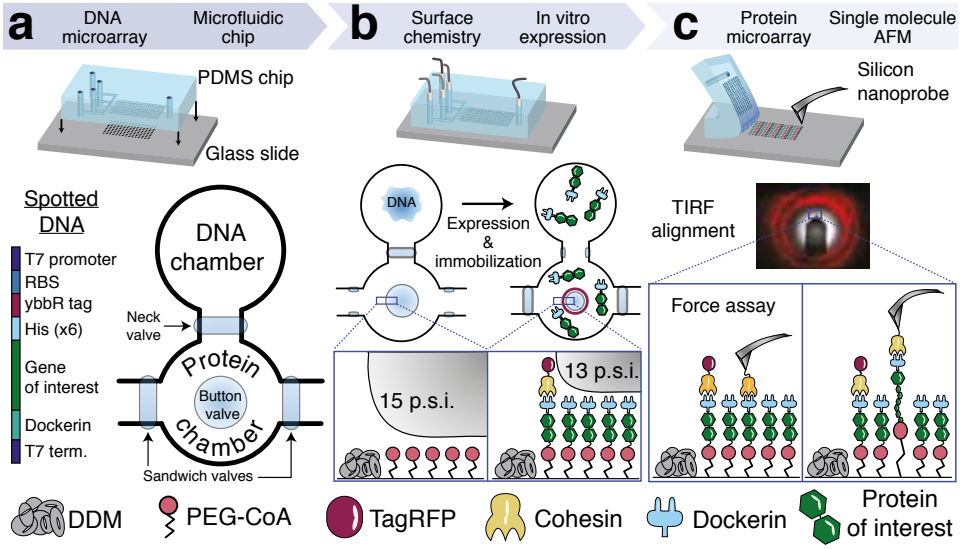
Mechanical forces acting on proteins play a pivotal role in biological systems. By applying forces to single molecules, conformational changes and energetic barriers along unfolding pathways can be probed by SMFS. Since low experimental throughput has significantly limited the capacity to screen libraries of proteins, we developed a versatile microfluidic system to address these issues. Our platform enables parallelized force spectroscopy utilizing cell-free in vitro gene expression, covalent protein immobilization and subsequent measurements of mechanical properties at the single molecule level in a streamlined format with one single cantilever. A PDMS microfluidic chip on a glass slide seals engineered DNA spots to provide micro reactors for protein synthesis. Expressed fusion proteins covalently attach to the glass surface at their N-termini and display free dockerin domains at their C-termini. With a single cohesin-functionalized cantilever, unfolding pathways and unbinding characteristics of multiple different proteins can be probed. Our example library contained structural proteins, cytoskeletal constituents, enzymes, and fluorescent proteins, which we were able to detect by their specific unfolding fingerprints. Analysis of contour-length increments and rupture force - loading-rate data characterizes the constructs and are compared with computational methods. As an application of this novel system, mutant variants of individual receptor-ligand proteins can be constructed, immobilized and measured on a single molecule basis to screen for candidates in protein design. For example, saturation mutagenesis of single residues responsible for binding their counterpart can be performed and characterized on a single device. This method provides a unique means of comparing forced dissociation and unfolding pathway characteristics of engineered proteins.



Method workflow. (a) A gene array is spotted onto a glass slide and a multilayer microfluidic chip featuring 640 unit cells is aligned to the DNA microarray and bonded to the glass slide. Each unit cell comprised a DNA chamber, a protein chamber, and superseding elastomeric control valves actuated by pneumatic pressure. (b) Control valves are utilized for spatially selective surface modification of each protein chamber with PEG-CoA, for fluidic isolation of each chamber prior to in vitro expression of the microspotted DNA and for fluorescent labeling with TagRFP-Cohesin. (c) After removal of the microfluidic device, the resulting well-defined, covalently attached protein microarray are accessed from above with a functionalized AFM cantilever. Single-molecule unfolding traces of each of the protein constructs are thus acquired sequentially at each corresponding array address with a single cantilever in a single experiment.

High Throughput Analysis of Bacterial Interactions

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Our goal is to understand interactions within bacterial communities. As antibiotic resistances of bacteria increase, one potential approach to fight harmful bacteria is to exploit the ability of natural communities to suppress invaders. Therefore, it is essential to understand bacterial interactions. In our approach, we focus on small model systems to understand the basic principles of bacterial interactions. We use the ColicinE2 system of *E.coli* and analyze its population dynamics via automated high throughput fluorescence microscopy. A novel aspect of our method is to use a zooming function in order to capture the population's growth dynamics over multiple spatial scales: from the single cell (microscopic) to the whole population (macroscopic) level. The bacterial system contains 3 competing bacterial strains: a toxin producing(C) strain, and strains sensitive(S) and resistant(R) to the toxin. It has been previously used as a model system in ecological studies of rock paper scissor games that are investigated both experimentally and theoretically. Here we show that, depending on environmental conditions, the system exhibits a variety of outcomes ranging from coexistence of at least two strains over survival of just one strain to no survival at all. This study provides new insights into the determinants of these outcomes.

Hierarchical and reversible assembly of shape-complementary non-basepairing DNA components

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In Nature, nucleic acid molecules can also recognize and bind ligands through weaker interactions than basepairing, which enables turnover and conformational dynamics on biologically relevant timescales. Such recognition occurs for example between RNase P, an RNA based enzyme, and its substrate, pre-transfer RNA (tRNA) (Fig. 1a). Here, we imitate the principle by which RNase P recognizes tRNA using programmable self-assembly with DNA to produce discrete, shape-complementary 3D compo-

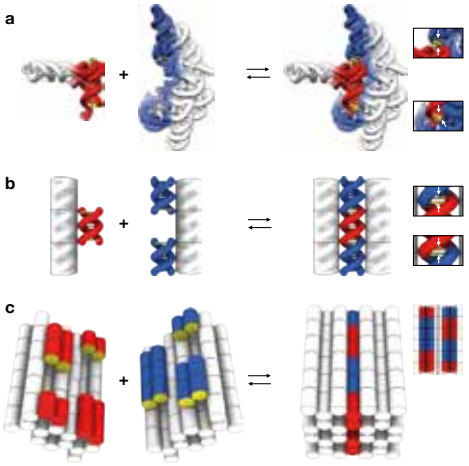

Figure 1: a) Illustration of the mechanism by which RNase P (blue / gray) recognizes tRNA (red / grey) b and c) Schematic representation of RNAse-P inspired click-in shape recognition between complementary DNA components. Cylinder elements indicate double-helical DNA domains that are one helical turn long. Inset in c highlights the precise fit of the shape-complementary patterns of double-helical DNA protrusions and recession.

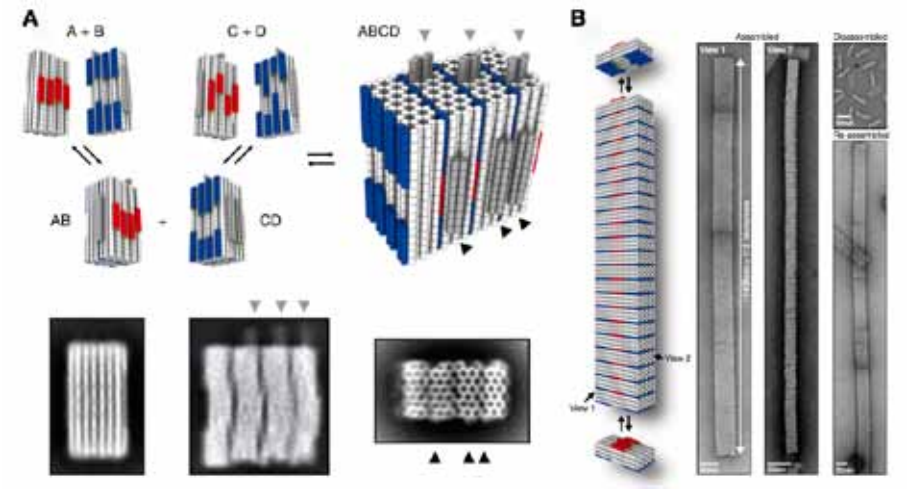

Figure 2: a and b) Schematic representation of four shape-complementary, orthogonal multi-layer DNA origami bricks. Average negative-stain TEM micrographs of the self-assembled DNA tetrameric object ABCD. Scale bar: 25 nm **c and d)** Schematic representation of filaments formed by cation-dependent reversible multimerization of a self-complementary multi-layer DNA origami brick. Negative-stain TEM micrographs showing typical filaments that grow and shrink in the presence different $MgCl_2$ concentrations. Scale bar: 50 nm

nents that interact via short-ranged nucleobase stacking bonds. To prove the concept of the RNase-P inspired shape recognition scheme we designed four multi-layer DNA origami bricks (Fig. 2a,b). The bricks form the subunits of a tetrameric complex and a combinatorial set of shape-complementary double-helical DNA domain protrusions and recessions. The contact interactions between shape-complementary interfaces also enable the reversible long-range assembly of DNA objects. For example, a self-complementary brick may be self-assembled into homomultimeric filaments with apparently seamless integration of up to hundreds of monomers (Fig. 2c). Simply decreasing or increasing the cation concentration allows recovering the constituent monomers or restoring the growth of filaments, respectively (Fig. 2 c,d). The absence of significant bending deformations up to the micrometer-length scale supports the notion of tightly bound states constrained by rigid lock-and-key type interfaces.

Probing the Conformational Dynamics of Proteins with High Multiplexed Magnetic Tweezers

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Magnetic Tweezers (MT) are a single molecule technique that enables the application of both forces and torques to biological macromolecules such as DNA or proteins. The molecules of interest are attached with one end to superparamagnetic beads, while their opposite ends are attached to the bottom surface of a flowcell. Magnets, placed above the flowcell, exert magnetic fields such that a constant force is applied to the molecules, without the need for feedback. Camera-based tracking is used to monitor the (x,y,z)-positions of the beads. Recent improvements in CMOS technology make it possible to track many beads at the same time, enabling us to perform multiple (currently up to ~200) single molecule measurements in parallel to address challenging biological questions with large statistical data sets. Alternatively, a reduced field of view can be used which enables fast measurements with frames rates in the kHz regime. Here, we present force clamp measurements of proteins. Using the instrument in the high-multiplexed-tracking mode, we are exploring the general requirements for protein unfolding measurements in MT, such as passivation of the surface, attachment strategies to bind the proteins to the surface as well as to the beads, and the right concentration of functional proteins bound to the surface. In our proof-of-concept measurements, we are investigating Green-Fluorescent-Protein (GFP) unfolding events to use as a fingerprint for future measurements of force clamp force-activation and unfolding of functional protein.

3D Real-Time Orbital tracking in zebrafish embryos: High spatiotemporal analysis of mitchondrial dynamics in neurons

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The main function of mitochondria is to provide cells with adenosintriphosphate (ATP) in regions with high-energy demand. A complex machinery of motor proteins (kinesin, dynein, myosin, etc.) and signaling molecules are responsible for the distribution and recycling of mitochondria in cells. A malfunction in the dynamics of these complexes is one possible reason for neurodegenerative diseases. To follow the trajectory of individual mitochondria in rohon-beard sensory neurons, we use a home-built three-dimensional real-time orbital-tracking microscope with a spatial resolution of a few and an acquisition speed of up to 500 Hz. Environmental information is recorded simultaneously with a built-in widefield microscope. By using photoactivation, we are able to track single mitochondria over distances of more than 100 µm. Due to our high spatial and temporal resolution, we can identify several different dynamic populations involved in mitochondrial transport. The

environmental information gives insight into the interactions between stationary and moving mitochondria. Combining the results from the fast and precise tracking microscope with the widefield data we obtain an in vivo overview over the dynamic processes in rohon-beard sensory neurons which can be used to study the effects of neurodegenerative diseases.

Manipulation of Plasmonic Nanoparticles by Optically Driven Thermal Convection

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We present an all-optical approach to move and manipulate single gold nanoparticles with high accuracy by thermal convection. The irradiation of an aqueous polymer solution with a focused laser beam leads to the formation of far-ranging thermal gradients. Particles that are suspended in such an environment are subject to thermophoretic and convective forces. The relative strengths of these forces depend mostly on physical parameters, such as the viscosity and the absorption coefficient of the medium. Here, we show how optically driven thermal convection can be employed to manipulate nanoparticles in an aqueous polyethylene glycol solution by looking at a regime where convective forces are dominant, while thermophoretic forces are negligible. We demonstrate how a single laser beam can be employed to control the movement of individual particles in 2D and 3D with nanoscale precision. The usage of multiple beams then reveals the entire potential of the approach, as it enables us to guide particles along arbitrary contours and curves. These results form a basis for understanding how thermal convection and can be used for further application in nanoscale physics, such as, for example, the exact positioning nano-sensors in biological systems.

Nanostructured lithium cobalt oxide for electrochemical lithium insertion

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The growing markets for electric vehicles and mobile electronics motivate the development of electrochemical energy storage systems with both high energy density and high power. Currently, two basic technologies are used to address, albeit partially, those needs. Supercapacitors can deliver very high powers, but their attainable energy densities are far lower than those of batteries. "Closing the gap" between the two main technologies requires the development of materials that can incorporate or liberate a large amount of charge in a very short time. Nanoscaling is a promising and intensively explored strategy to maximize the rate performance of battery materials. Reducing the crystal size down to just a few nanometers greatly increases the interface, leading to enhanced charge transfer and drastically shortens the ion/electron diffusion pathways compared to bulk material, thus providing electrochemical energy storage systems with both high energy density and high power. Nanoscaling is therefore one of the perspective directions in the development of efficient electrochemical energy storage systems. We develop new pathways for the fabrication of different ternary metal oxide nanoparticles for the application in lithium-ion batteries. Furthermore, our research focuses on controlled assembly of nanocrystals into continuous networks providing charge transfer junctions with high interface area and a continuous pathway for the charge transport. Aiming to prepare metal oxide nanoparticles of small size, enhanced crystallinity and good dispersibility, we explored tert-butanol as a novel reaction medium. Using this method we were able to obtain fully crystalline interconnected porous frameworks composed of ultrasmall titania (TiO_2) and lithium titanate $Li_4Ti_5O_{12}$ (LTO) spinel nanocrystals, which were shown to be the fastest ever-reported titanate morphologies as anode materials for lithium insertion.[1,2] We have found that the reduction in crystal size also leads to a change in bulk ion transport properties of the nanocrystals, explaining their extremely fast electrochemical lithium insertion rates. Here we show the extension of our successful synthesis strategy to the development of nanostructured thin films of lithium cobalt oxide $LiCoO_2$ (LCO), which was the first commercially used cathode material in lithium ion batteries. The reduction in size leads to faster charge and discharge processes in nanostructured LCO compared to bulk material.

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Femtonewton resolved determination of optical forces acting on a single gold nanoparticle

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Optomechanical manipulation of plasmonic nanoparticles is an area of current interest that has led to numerous applications in nanofabrication, sensing, analytics, biology and medicine.[1] However, no experimental method is available to quantitatively determine the forward-directed scattering force that dominates for incident light of a wavelength close to the particle plasmon resonance. Here, we demonstrate how the scattering force acting on a single gold nanoparticle in solution can be measured. We obtain a resolution of less than 8 femtonewtons which is a factor of three smaller than any measurement of switchable forces performed on nanoparticles in solution with single beam optical tweezers to date. An 80 nm gold nanoparticle is optically trapped in water by 1064 nm focused laser light and observed using dark field microscopy. Via an optical single mode fiber oriented perpendicularly to the trapping beam, it is then exposed to chopped, 532 nm laser light being resonant with the plasmon frequency. A thorough analysis of the power spectral density of the particle movement[2] provides an analytical value for the scattering force. We compared the results of our force measurement with Mie simulations of the optical force on a gold nanoparticle and found good agreement between experiment and theory.[3] The accuracy of this novel method for force measurements lies within a few fN.

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Measuring intra-molecular distances by anomalous small-angle x-ray scattering

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Measurements of molecular distances are key to dissect the structure, dynamics, and functions of biological macromolecules. While FRET and NMR-based techniques have provided invaluable details by measuring intra-molecular distances, they suffer from a limited range (< 10 nm) and difficulties in converting the measured signal into absolute distances. SAXS measurements employing gold-nanoclusters as labels on DNA constructs have demonstrated their ability to provide information about the entire gold label-gold label distance distribution for a considerable range of distances. The distance distributions are obtained by inverting the gold label-gold label scattering interference term. So far, two approaches have been employed to separate the label-label interference terms from the other contributions (intra-label, label-macromolecule, and intra-macromolecule) to the measured scattering profile. Firstly, the single-labeled and unlabeled samples were measured in addition to the double-labeled macromolecules and from addition and subtraction of the appropriate profiles the interference term could be determined. A second approach relies on using relatively large (~ 5 nm) gold particles and neglecting the DNA and gold-DNA scattering terms. However, both approaches have some specific drawbacks. Here, we demonstrate measurement of intra-molecular distances on 10, 20, and 30 bp DNA constructs carrying two small (~1 nm) gold labels using anomalous small-angle X-ray scattering (ASAXS). Our approach only requires the double-labeled samples and relies on recording scattering profiles for each sample at different energies. By tuning the X-ray energy through the gold L-III edge (at ~11.9 keV), it is possible to separate out the gold contributions from the DNA only and gold-DNA scattering terms. Our results demonstrate that ASAXS based determination of label-label distances is possible and provides an attractive alternative to determine absolute intra-molecular distance distributions.

Modeling bacteria-phage relationship in complex communities—oral biofilms

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Bacterial biofilms are aggregates of bacteria in which cells adhere to each other or to a surface. In many areas of human activity such as water treatment, food safety, and medical implants, biofilm formation is deleterious. Formation is sequential and highly structured, necessitating community action and extracellular matrices that persist throughout the duration of the biofilm, which can make penetration extremely difficult. The community action of some bacteria enables disease initiation and progression whereas free-floating bacteria do not. Long-standing biofilms of pathogenic bacteria can therefore lead to serious consequences for consumers and patients. Bacteriophages are microorganisms that adsorb onto and inject their genetic material into bacterial cells. Phages may choose the destructive lytic life cycle or the lysogenic life cycle. In isolated strains of bacteria, phages often lyse their hosts when hosts are unable to sustain stable growth. In a highly structured community of bacteria, interaction between phages and their hosts is not well understood. Understanding this interaction on a community level may give insight into treatment of biofilm-generated diseases. A model for such biofilms is needed. In this study, we choose the dental surface as the model environment for biofilm study. Our goal is to mimic the tooth enamel and the passage of saliva over this surface in order to build an in vitro model to study bacteria-phage interactions. We use clarified saliva to form the pellicle, basal mucin medium to grow bacteria, and dental plaque samples to seed the biofilms. Our preliminary results show steady growth of biofilms over a 24-48hr period without need for extensive instrumentation.

MOF-Based Core-Shell Nanoparticles for Biomedical Applications

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Metal-organic frameworks (MOFs) are a class of porous materials that have attracted increasing interest in recent years. The ability to adjust pore sizes and to implement functionalities within the pores enhances their potential, especially in comparison with classical porous solids. Thus, MOFs are envisioned as promising candidates for drug delivery nanocarriers.[1] Such nanocarriers (diameter 20 – 200 nm) are porous materials that are suitable for an efficient and targeted delivery of biologically active molecules. For this purpose synthetic strategies for the generation of well-defined functional MOF nanoparticles are needed. Here we focus on the external surface functionalization of MIL-100(Fe) nanoparticles, intending their use as drug delivery vehicles. The synthesis was carried out under optimized hydrothermal conditions following literature procedures.[2,3] The resulting particles exhibit attractive properties such as large surface area, high crystallinity, chemical stability, and a fairly narrow size distribution (approx. 50 – 150 nm). Covalent surface functionalization of the particles with different polymer chains (Polymer@MOF) was performed by a catalyzed amidation reaction and the successful bond formation was confirmed by liquid state NMR spectroscopy. By covalently attaching a polymer shell, we were able to implement different functionalities onto MIL-100(Fe) nanoparticles that are of interest regarding stability and drug delivery requirements. The shell, consisting of a well-defined multifunctional polyamine showed high potential for siRNA binding. This was confirmed by gel-electrophoresis experiments. Cell experiments showed low toxicity and successful uptake of our siRNA-loaded polymer-functionalized particles. These results are promising steps towards functional MOF nanoparticles that are suitable as nanocarriers in biomedical applications.

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Simoncelli	Sabrina	LMU Munich
Stadler	Katharina	LMU Munich
Stamp	Melanie	University of Augsburg
Stefani	Fernando	University of Buenos Aires
Stolarczyk	Jacek	LMU Munich
Sudhop	Stefanie	University of Applied Science Munich
Tong	Yu	LMU Munich
Trauner	Dirk	LMU Munich
van Oijen	Antoine	University of Wallongong
Vanderlinden	Willem	LMU Munich
Veigel	Claudia	LMU Munich
Verdorfer	Tobias	LMU Munich
Vogel	Horst	EPFL
von Bronk	Benedikt	LMU Munich
Wagenbauer	Klaus	TU Munich
Walker	Philipp	LMU Munich
Wehnekamp	Fabian	LMU Munich
Weitz	Thomas	BASF SE Ludwigshafen
Weller	Horst	Universität Hamburg
Winterer	Felix	LMU Munich
Wittmann	Christoph	University of Augsburg
Zareva	Michaela	LMU Munich
Zehetmaier	Peter	LMU Munich
Zensen	Carla	LMU Munich
Zettl	Thomas	LMU Munich
Zhou	Baoqing	UC Santa Barbara
Ziegler	Daniela	TU Munich
Zimpel	Andreas	LMU Munich

Accommodation

Accommodation for all participants is provided on San Servolo. The buildings are situated in the island's beautiful green parkland. All bedrooms have air conditioning, television, telephone and internet access. A twenty-four hour reception service is guaranteed.

Welcome Reception

The Welcome Reception will take place on Sunday, Sept. 20, at about 8:00 pm on San Servolo in Sala Grecale (building 11).

Breakfast and lunch

The cafeteria is located on the ground floor of building 15. The cafeteria is open every day with the following timetable:

Breakfast	7.30 am - 9.30 am
Lunch	12.00 pm - 2.30 pm
Dinner	7.00 pm - 9.15 pm

For participants with accommodation on San Servolo, breakfast is included (*please sign for your breakfast at the list at the counter in the cafeteria*). Prices for lunch or dinner are € 11.00 and include a pasta course, a main course, a side order of vegetables or salad, yoghurt, bread and water. There are also reduced menus available (pasta course, side order of vegetables or salad, water and bread, or: main course, side order of vegetables or salad, water and bread).

A coffee bar offering snacks and warm and cold beverages is also available on campus and is located on the ground floor of Area 6 in the main building. The coffee bar is open from 7.50 am to 5.50 pm.

For self-catering, supermarkets are located close to the boat stops Piazzale de Roma and Zattere.

Internet

All hotels room on San Servolo have WLAN access. In addition, there will be a conference WLAN in the lecture hall.

WLAN Conference Network San Servolo: UNIVIU

username: censworkshop2015
password: censworkshop2015

Internet activity will be monitored and recorded as required by Italian law.

Timetables

TRAIN TO VENICE AND BACK TO MUNICH

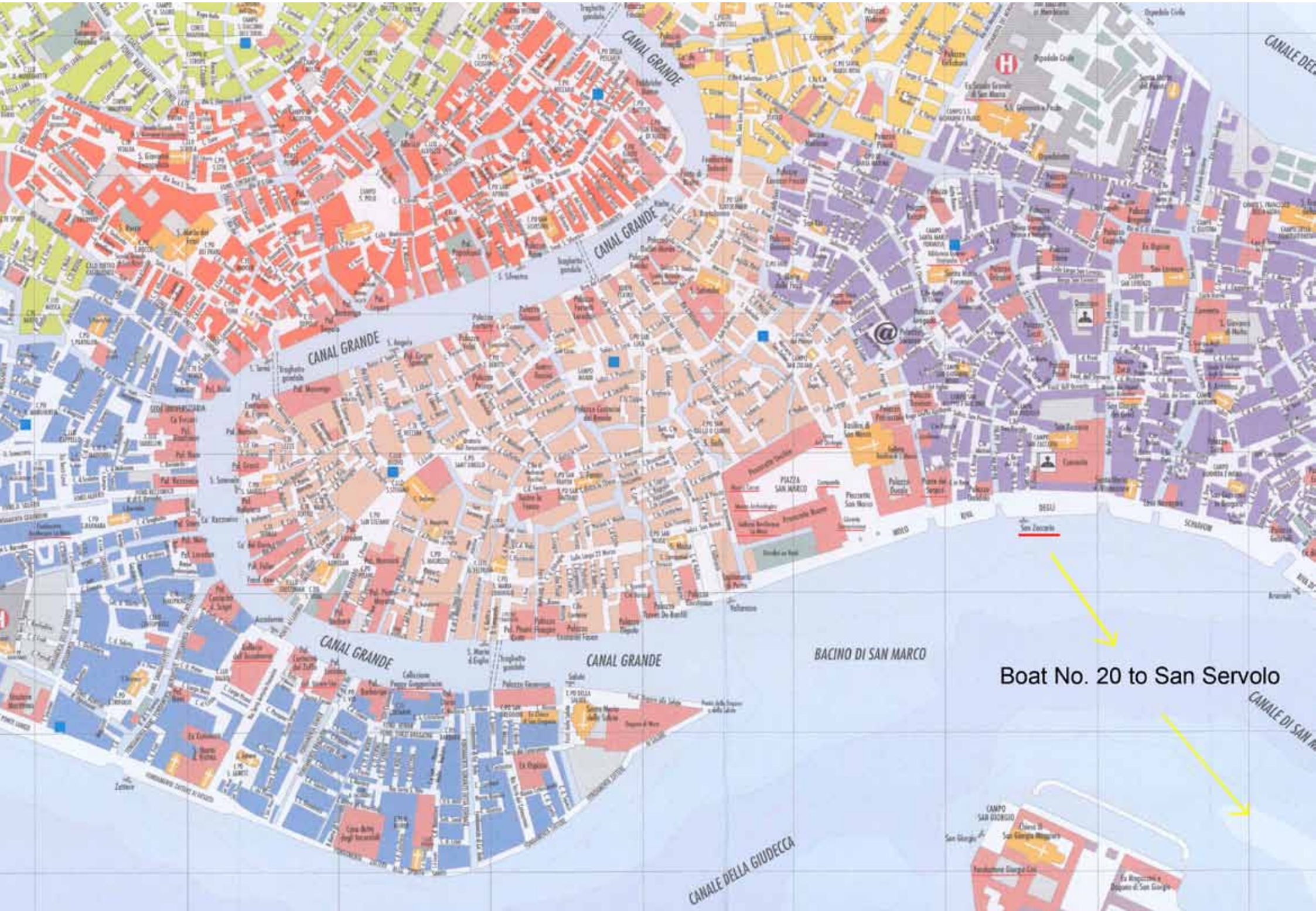
To Venice (20.09.)		Back to Munich (25.09.)	
Munich Main station	**Venezia Santa Lucia**	**Venezia Santa Lucia**	**Munich Main station**
11:35	18:10	13:35	20:21

BOAT LINE 20 TO WORKSHOP LOCATION (SAN SERVOLO)

The boat from Venice to San Servolo leaves from the Riva degli Schiavoni at San Marco/San Zaccaria; the stop is in front of the Londra Palace Hotel. Boat number 20 goes to San Servolo.

To San Servolo		Back to Venice	
S. Zaccaria	**S. Servolo**	**S. Servolo**	**S. Zaccaria**
6:55	*7:05*	*7:05*	*7:15*
7:15	*7:25*	*7:35*	*7.45*
8:10	*8:20*	*8:30*	*8:40*
8:40	*8:50*	*8:50*	*9:00*
9:00	*9:10*	*9:10*	*9:20*
9:20	*9:30*	*9:40*	*9:50*
9:50	*10:00*	*10:00*	*10:10*
10:30	*10:40*	*10:50*	*11:00*
11:10	*11:20*	*11:20*	*11:30*
11:50	*12:00*	*12:10*	*12:20*
12:30	*12:40*	*12:40*	*12:50*
13:10	*13:20*	*13:30*	*13:40*
13:50	*14:00*	*14:00*	*14:10*
14:30	*14:40*	*14:50*	*15:00*
15:10	*15:20*	*15:30*	*15:40*
15:50	*16:00*	*16:00*	*16:10*
16:30	*16:40*	*16:50*	*17:00*
17:10	*17:20*	*17:30*	*17:40*
17:50	*18:00*	*18:00*	*18:10*
18:30	*18:40*	*18:50*	*19:00*
19:10	*19:20*	*19:20*	*19:30*
19:50	*20:00*	*20:00*	*20:10*
20:30	*20:40*	*20:40*	*20:50*
21:30	*21:40*	*21:40*	*21:50*
22:30	*22:40*	*22:40*	*22:50*
23:30	*23:40*	*23:40*	*23:50*
0:25	*0:35*	*0:35*	*0:45*
1:20	*1:30*	*1:30*	*1:40*

Remember to arrive a few minutes before departure time.


CANAL GRANDE
CANAL GRANDE
CANAL GRANDE
CANAL GRANDE
BACINO DI SAN MARCO
CANALE DELLA GIUDECCA
PIAZZA SAN MARCO
San Zaccaria
Boat No. 20 to San Servolo
CANALE DI SAN

CeNS Workshop Venice: Channels and Bridges to the Nanoworld

Time	Monday, September 21
09:00	**Welcome**
09:15	**Antoine van Oijen** Molecular choreography on a tightrope: a single-molecule view of DNA replication
10:00	**Klaus Müllen** Carbon nanostructures as func-tional multitalents - sensing, cata-lysis, drug delivery, electronics
10:45	**Coffee break**
11:15	**Aurora Manzi** Light-induced cation exchange for copper sulfide based CO_2 reduction
11:35	**Roland Beckmann** title tba
	Lunch (12:20-14:15)
14:15	**Michael Gordon** Manipulating light with nanostructures: controlling reflection to chemical imaging
15:00	**Sheref Mansy** Cell-free genetic systems for the construction of cellular mimics
15:45	**Coffee break**
16:15	**Victor Brar** Electrostatically tunable meta-surfaces for controlling optical wavefronts and thermal emission
17:00	**Thorben Cordes** Mechanisms of membrane transport: a single-molecule view on ABC importers

Time	Tuesday, September 22
09:00	**Horst Weller** Tailor-made synthesis & ligand design for the use of nanocrystals in materials- & life science applications
09:45	**Chase Broedersz** Breaking detailed balance at the mesoscale in active biological systems
10:30	**Coffee break**
11:00	**Horst Vogel** Ligand-gated ion channels: From 3D structure to transmembrane signaling
11:45	**Theobald Lohmüller** Thermoplasmonic control of chemical reactions and cell function at the nanoscale
	Lunch (12:30-14:15)
14:15	**Thomas Weitz** Organic electronics: fundamentals and applications of organic field-effect transistors in flexible displays
	Posters session I **&** **coffee** **(15:00-17:00)**
17:00	**Fernando Stefani** Manipulating light, heat and forces at the nanoscale with metallic nanoparticles
17:45	**Omar Saleh** Polymer mechanics across the force regimes

Time	Wednesday, September 23
09:00	**Yifan Cheng** TRP channel structures by single particle cryo-EM - from blob-ology to atomic structures
09:45	**Melike Lakadamyali** Decoding chromatin organization with super-resolution microscopy
10:30	**Coffee break**
11:00	**Matthias Scheffler** Big-data analytics for materials science: concepts, challenges, and hype
11:45	**Eva Nogales** Cryo-EM studies of complex systems: microtubule Dynamics and Transcription Initiation
	Lunch (from 12:30) Boat from San Servolo at 12:40 and 13:30
	Informal discussions

Time	Thursday, September 24
09:00	**Stefan Raunser** Structural insights into life and death of a bug
09:45	**Thomas Klar** From STED microscopy to STED lithography
10:30	**Coffee break**
11:00	**Ebbe Andersen** Principles of biomolecular design
11:45	**Ulrich Schollwöck** Improving material simulations with the dynamical mean-field theory
	Lunch (12:30-14:15)
14:00	**Tim Clark** Simulating organic and hybrid electronic devices
	Posters session II **&** **coffee** **(15:00-17:00)**
17:00	**Andrew Ellington** Developing chemical reaction network computers
17:45	**Diana Pippig** Molecular tools for advanced single-molecule studies

Time	Friday, September 25
09:00	**Jörg Hartig** Engineered ribozymes assynthetic genetic switches
09:45	**Deborah Fygenson** DNA nanotube nucleation: how it happens and what it can do for you
10:30	**Closing remarks & coffee**
	Boats to San Zaccaria leave at 10:50 / 11:20 / 12:10 Train to Munich leaves at 1:35 pm from Venice train station