CeNS
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## CeNS Workshop 2010

# Nanosciences: Merging Disciplines

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## Content

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# Invited Talks

## Enhancing and localizing light-matter interaction using optical antennas

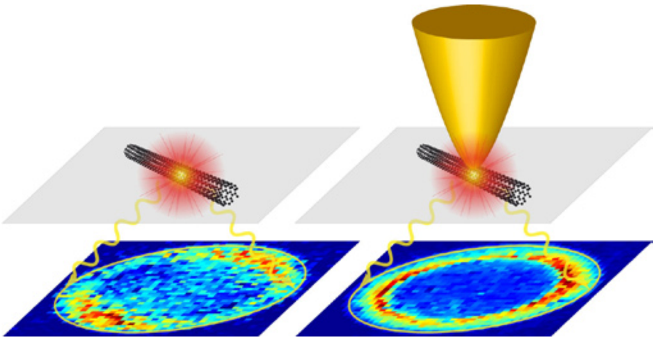
**Achim Hartschuh**

*Department Chemie and CeNS, Ludwig-Maximilians-Universitaet Muenchen, Germany*

An antenna couples free propagating electromagnetic radiation to a local receiver or transmitter. In the optical regime such a receiver / transmitter could be formed by a single chromophore or a semiconductor nanocrystal and the near-field of an antenna can be used to locally enhance the absorption and emission rates of these quantum structures. Prominent examples utilizing antenna phenomena in the visible range include surface enhanced Raman scattering and surface enhanced fluorescence. Control of light-matter interaction is also becoming relevant for improving device characteristics in optoelectronics and photo-voltaics.

Raster-scanning the antenna across the sample surface in so called tip-enhanced near-field optical microscopy (TENOM) provides ~10 nm spatial resolution and increased detection sensitivity [1]. Since high spatial resolution is a result of local signal enhancement, this approach is ideally suited for studying very weak optical responses such as Raman scattering and fluorescence from low-quantum yield emitters.

We present recent TENOM studies of single carbon nanotubes and semiconductor nanowires and show that antenna coupling leads to an angular redirection of emission (Figure, [2]). We then illustrate a new strategy for shaping optical near-fields that combines concepts and tools of ultrafast spectroscopy with those of optical antennas is illustrated [3].



Radiation pattern detected for a single photoluminescent nanotube with and without optical antenna.

*[1] A. Hartschuh, "Tip-enhanced near-field optical microscopy", Angew. Chemie 47, 8178 (2008)*

*[2] M. Böhmler et al., "Enhancing and redirecting carbon nanotube photoluminescence by an optical antenna", Optics Express 18, 16443 (2010)*

*[3] G. Piredda et al., "Controlling near-field optical intensities in metal nanoparticle systems by polarization pulse shaping", Appl. Phys. B 100, 195 (2010)*

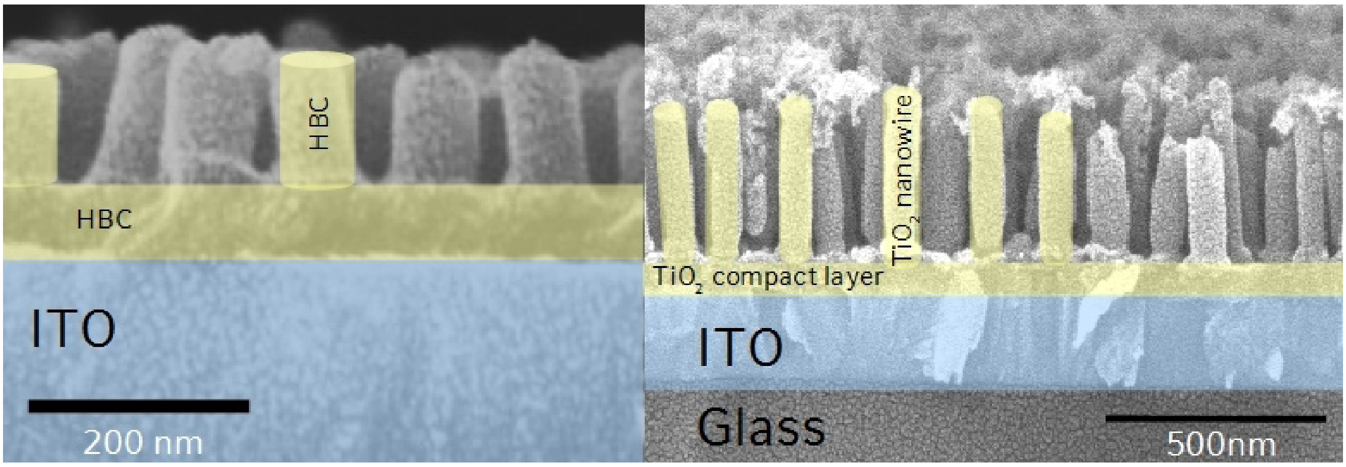
## Nanostructured Organic and Hybrid Solar Cells

**Lukas Schmidt-Mende**

*Ludwig-Maximilians-University (LMU) Munich, Dept. of Physics & Center for NanoScience (CeNS)*

Morphology control is a key issue towards more efficient organic solar cells. However, it is difficult to achieve the desired control in purely organic materials. In this presentation several approaches towards control of nano-morphology in organic and hybrid solar cells will be discussed. Nano-imprint methods can lead to nanostructured organic solar cells [1]. Metal-oxide nanostructures are used as template and combined with organic materials for hybrid solar cells. Novel fabrication methods allow the controlled fabrication of structures in nanometer size designed for solar cell applications. Promising approaches and their advantages will be discussed with emphasis on their potential in future applications.

*[1] W. Wiedemann, L. Sims, A. Abdellah, A. Exner, R. Meier, K. P. Musselman, J. L. MacManus-Driscoll, P. Muller-Buschbaum, G. Scarpa, P. Lugli, L. Schmidt-Mende, Applied Physics Letters 2010, 96, 263109.*



Two examples for nanowires arrays on conducting glass substrates: Left: imprinted organic hexabenzocoronene, Right: $TiO_2$.

## Molecular and cellular studies of dynamical networks in translation

**Zan Luthey-Schulten**

*Department of Chemistry, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*

Signaling pathways in RNA:protein complexes involved in translation are identified by community network analysis derived from molecular dynamics simulations. These complexes include the amino-acyl-tRNA synthetases, which set the genetic code by charging tRNAs with their cognate amino acids, the elongation factor EF-Tu, which transports the charged tRNAs to the ribosome, and the ribosome, which is the site of protein synthesis. A dynamic contact map defines the edges connecting nodes (amino acids and nucleotides) in the physical network whose overall topology is presented as a network of communities, local substructures that are highly intraconnected, but loosely interconnected. While nodes within a single community can communicate through many alternate pathways, the communication between monomers in different communities has to take place through a smaller number of critical edges or interactions which are evolutionarily conserved. The time dependent variation of these networks during tRNA migration is consistent with kinetic data and reaction mechanisms suggested at each step of translation.

In bacterial cells, translation involves thousands of these RNA:protein complexes which occupy a large portion of the cell volume and make a major contribution to the extrinsic noise of gene expression. Using data from proteomics, cryo-electron tomography, and *in vivo* single molecule fluorescence experiments, we study the inducible lac genetic switch in a modeled E. coli cell. Compared to models in which the spatial heterogeneity is ignored, the in vivo model predicts an overall lowering of cellular noise, due to the influence of molecular crowding on transcription factor binding rates. To address the problem of performing long time simulations of biochemical pathways under in vivo cellular conditions, we present a lattice-based, reaction-diffusion model that runs on graphics processing units (GPUs).

*[1] "Experimental and computational analysis of tRNA dynamics", R. Alexander, J. Eargle, and Z. Luthey-Schulten, FEBS Letters, 584 (2), 376-386 (2010)*

*[2] "Dynamic Networks: Signaling Pathways in Protein/tRNA Complexes" , A. Sethi, J. Eargle, A. Black, and Z. Luthey-Schulten, Proc. Natl. Acad. Sci. USA, 106, 6620-6625 (2009)*

*[3] "Long time-scale simulations of in vivo diffusion using GPU hardware", E. Roberts, J. Stone, L. Sepulveda, Wen-mei Hwu, and Z. Luthey-Schulten, in Proceedings 8th IEEE International Meeting on High Performance Computational Biology, (2009).*

## DNA Origami and DNA Tensegrity

**Tim Liedl**

*Faculty of Physics and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München*

I will describe our current research based on DNA origami [1] and discuss the possibilities arising with this recent method, which allows the construction of arbitrary three-dimensional DNA objects [2] that can be addressed with a wide variety of functional groups at nanometer precision. Further, the design of prestressed DNA tensegrity structures will be highlighted. Prestressed tensegrity structures exhibit compression resistant elements connected by tension bearing components, such as strings or springs. Such tensed networks have the ability to adsorb distortions and propagate them over the whole structure and self-stabilize into their original shapes after the distortion is relieved [3]. We built nanoscale 2D and 3D prestressed tensegrity objects assembled from rigid multi-helical DNA bundles (resistant to compression) connected by single-stranded DNA acting as entropic springs (bearing tension) [4]. The tension provided by the single-stranded DNA springs can be high enough to bend rigid DNA six-helix bundles.

One reason for the scientific interest in this design principle is the underlying potential to build large objects of great overall stability while using relatively small amounts of building material. On the other hand, the concept of tensegrity has helped to understand the physical behavior of viruses, cells, tissues, organs and organisms from the nano to the macro scale [5].

*[1] Rothemund, P.W.K.,'Folding DNA to create nanoscale shapes and patterns', Nature 440, 287-302 (2006)*

*[2] Douglas, S. M. et al. 'Self-assembly of DNA into nanoscale three-dimensionalshapes'. Nature 459, 414–418 (2009).*

*[3] Buckminster Fuller, Synergetics-Explorations in the Geometry of Thinking, Volumes I & II, New York, Macmillan Publishing Co, (1975, 1979)*

*[4] Liedl, T. et. al. 'Self-assembly of three-dimensional prestressed tensegrity structures from DNA', Nature Nanotechnology 5, 520-524 (2010).*

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## Live-cell imaging and single-particle tracking of polyplex internalization

**Nadia Ruthardt**

*Ludwig-Maximilians-University Munich & Center for NanoScience (CeNS)*

Systemic delivery of therapeutic genes for gene therapy or cancer gene therapy requires gene vectors that overcome several barriers. The vector has to enable tissue-selective delivery, internalize efficiently and finally release its cargo reliably within the target cell. Tissue specificity and enhanced internalization can be achieved by cell specific ligands that bind to certain surface markers which are upregulated in e.g. solid cancers. Functionalization with pH- and redox-sensitive linkers or polymers allows the vector to "sense" external stimuli which will trigger their activation in temporally and spatially controlled manner.

We investigate the uptake of targeted and untargeted polymeric gene vectors (polyplexes) by highly sensitive fluorescence microscopic methods on a single cell level [1]. The epidermal growth factor receptor (EGFR) is overexpressed on a high percentage of human carcinomas and is therefore an attractive therapeutic target for tissue-specific targeting by non-viral vectors in cancer gene therapy. By comparing uptake kinetics and internalization dynamics, single particle tracking in combination with quenching experiments revealed typical three-phase dynamics of the uptake process independent of targeting. Phase I was characterized by slow, actin-cytoskeleton-mediated movement of the particles with drift and included the internalization process. During phase II, particles displayed increased velocities with confined and anomalous diffusion in the cytoplasm. Phase III was characterized by fast active transport along microtubules. Targeting of polyplexes for receptor-mediated endocytosis by the EGF receptor resulted in shortening of phase I and strongly accelerated internalization. Targeted as well as untargeted particles were transported in early endosomes marked by Rab5-GFP and accumulated in late endosomes marked by Rab9-GFP.

The endosomal release dynamics of polyplexes consisting of DNA condensed with the cationic polymers linear polyethyleneimine (LPEI), poly-(L)-lysine (PLL) or poly-(D)-lysine (PDL) were studied by photochemical release in living cells [2]. Using double-labeled polyplexes, DNA and polymer were imaged simultaneously by dual-color fluorescence microscopy. Our results demonstrate that the characteristics of the cationic polymer significantly influence the release behavior of the polyplexes. For LPEI/DNA particles, LPEI quickly spread throughout the cytosol, whereas DNA was released slowly and remained immobile thereafter. In case of PLL particles, both DNA and polymer showed quick release. PDL particles remained condensed upon photosensitizer activation.

*[1] K. de Bruin, N. Ruthardt, K. von Gersdorff, R. Bausinger, E. Wagner, M. Ogris, C. Bräuchle, Cellular dynamics of EGF receptor-targeted synthetic viruses, Mol Ther, 15 (2007) 1297-1305.*

*[2] K.G. de Bruin, C. Fella, M. Ogris, E. Wagner, N. Ruthardt, C. Bräuchle, Dynamics of photoinduced endosomal release of polyplexes, J Control Release, 130 (2008) 175-182.*

## In Control of Molecular Assembly & Motion

**Ben L. Feringa**

*Center for Systems Chemistry, Stratingh Institute for Chemistry & Zernike Institute for Advanced Materials University of Groningen, Nijenborgh 4, 9747 AG Groningen.*

Inspired by Nature we design nano-scale systems in which the control of dynamic properties of molecules is coupled to specific functions. Molecular machines ultimately require control over structure, organization and function of multi-component molecular assemblies at different hierarchical levels. Major challenges are the integration of kinetic driven processes in multifunctional molecular systems and control over translational and rotary motion.

Molecular switches and motors offer ample opportunity to control functions in a dynamic way. Following the development of the first light-driven unidirectional molecular motor, the focus is now on the control of dynamic functions in more complex systems as well as autonomous motion. Synthetic approaches to various molecular switches and motors and the construction of integrated systems featuring trigger and motor elements are discussed.

Specific challenges that we address are the acceleration of molecular rotary motors and the construction of a nanoscale "windmill park" powered by light. Recent advances in the design of new generation motors that allow the increase of the speed of rotation over a million fold are presented. Furthermore the design of molecular motors in which the rotary direction can be reversed, a molecular crankshaft and brake and molecular transmission phenomena are discussed. Besides rotary motion induced by light, we present unique molecular motors that run on a chemical fuel and discuss our attempts to achieve autonomous motion.

## Quantum Opto-Electronics with Semiconducting Nanowires and Carbon Nanotubes

**Leo P. Kouwenhoven**

*TU Delft, Quantum Transport Group*

We are interested in quantum controlling the optical and electronic behavior of solid state nanostructures. We are working towards an interface, based on pn-junctions, for transferring electronic quantum states coherently into photonic states. Our systems of choice are (InAsP) semiconducting nanowires and Carbon nanotubes. Both systems have been cleaned up such that we can control individual electrons and holes, study their hyperfine and spin-orbit interactions, control spin qubits and discover properties of mechanics at the nanoscale. The quantum behavior is measured both in electrical and optical properties.

## The Promise of Nano-Materials for Energy Related Applications

**Mildred S. Dresselhaus**

*Department of Electrical Engineering and Computer Science and Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA, http://mgm.mit.edu*

Energy security from renewable sources will be one of the major societal challenges of the 21st century. Nano-structured materials are expected to play a major role in addressing this challenge because materials at the nano-scale exhibit properties that are both different from what they are in their bulk form and because at a sufficiently small size the properties of a material become size dependent, thereby providing another handle for the control of its material properties. Goals for the mid-century are to be able to produce about 1.5 TW of power by photovoltaic technologies exploiting light from the sun and an equal amount of power by thermoelectric technologies exploiting heat provided by sunlight. Reaching these goals would require more than a 500-fold increase in photovoltaic power production and a 250-fold increase in thermoelectric power production. In this talk the role that nanoscience and nanotechnology is likely to play in meeting this challenge will be outlined in general terms for both the case of photovoltaics and thermoelectrics. A more detailed discussion will be presented for the case of thermoelectric energy production. Recent advances in the development of exciting new thermoelectric materials will be reviewed, including the scientific, industrial, and nanotechnology-based advances. Specific emphasis will be given to the special role that nanoscience plays in enabling nano-materials to provide size dependent materials properties that are especially favorable for enhancing thermoelectric performance because the control of nano-particle size makes it possible to decrease the thermal conductivity much more than the electrical conductivity, thereby providing a vivid example of the power of nanoscience and nanotechnology in enhancing thermoelectric materials performance.

## Designer cellulosomes as a viable macromolecular platform for the nanosciences

**Edward A. Bayer**

*Department of Biological Chemistry, The Weizmann Institute of Science, Rehovot 76100 Israel*

Cellulosomes are complex multi-enzyme machines produced by anaerobic cellulolytic bacteria, designed for efficient decomposition of plant cell wall polysaccharides, notably cellulose. This macromolecular complex consists of interlocking, multi-modular, structural and enzymatic subunits, which fit together like a molecular “Lego”. The key to cellulosome architecture is the arrangement of multiple *cohesin* modules on a central organizing *scaffoldin* subunit, to which the various enzymes are attached via complementary *dockerin* modules. We have harnessed the molecular logic of the cellulosome components and have developed methodologies to re-tool its precise structural organization. For this purpose, functional modular parts of cellulosome subunits from different microorganisms are mixed and matched by recombinant means to produce chimaeric products, which can be fitted together in a controlled manner into novel cellulosome-like structures, which we call “designer cellulosomes”. Using this approach, we can re-fabricate in a precise and exquisite manner the exact complement of desired components into highly uniform complexes. These artificial cellulosomes are functional in all their parts. In the case of cellulolytic enzymes, their capacities approach and frequently surpass those of equivalent free enzyme systems. This approach is designed to better understand the intercomponent interactions among cellulosomes, to discover how the cellulosome is constructed and how cellulosome architecture contributes to the enhanced synergistic activities of its enzyme components. Moreover, this system will allow restructuring of the components into unconventional (non-cellulolytic and non-enzymatic) macromolecular arrangements for alternative applications in the nanosciences.

*[1] Lamed, R., Setter, E. & Bayer, E. A. (1983). Characterization of a cellulose-binding, cellulase-containing complex in Clostridium thermocellum. J. Bacteriol. 156, 828-836.*

*[2] Bayer, E. A., Morag, E. & Lamed, R. (1994). The cellulosome — A treasure-trove for biotechnology. Trends Biotechnol. 12, 378-386.*

*[3] Fierobe, H.-P., Mechaly, A., Tardif, C., Belaich, A., Lamed, R., Shoham, Y., Belaich, J.-P. & Bayer, E. A. (2001). Design and production of active cellulosome chimeras: Selective incorporation of dockerin-containing enzymes into defined functional complexes. J. Biol. Chem. 276, 21257-21261.*

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*[6] Bayer, E. A., Lamed, R., White, B. A. & Flint, H. J. (2008). From cellulosomes to cellulosomics. Chem. Rec. 8, 364-377.*

*[7] Karpol, A., Kantorovich, L., Demishtein, A., Barak, Y., Morag, E., Shoham, Y., Lamed, R. & Bayer, E. A. (2009). Engineering a reversible, high-affinity system for efficient protein purification based on the cohesin-dockerin interaction. J. Mol. Recogit. 22, 91-98.*

*[8] Moraïs, S., Heyman, A., Barak, Y., Caspi, J., Wilson, D. B., Lamed, R., Shoseyov, O. & Bayer, E. A. (2010). Enhanced cellulose degradation by nano-complexed enzymes: Synergism between a scaffold-linked exoglucanase and a free endoglucanase. J. Biotechnol. 147, 205-211.*

## Quantum-Chemical Calculation of Intermolecular Interactions for Molecular Systems with 1000 and More Atoms

**Christian Ochsenfeld**

*Chair of Theoretical Chemistry, University of Munich (LMU) Butenandtstr. 7, D-81377 Munich, Germany*

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Quantum chemistry has evolved over the last decades to become a versatile tool for studying structures and properties of molecular systems. Despite this success, the applicability to large molecules is hampered by the strong polynomial increase of the computational effort with molecular size M. Therefore a central goal of our work is to overcome this scaling wall and to develop linear-scaling methods, which allow for quantum-chemical studies of molecular systems with 1000 and more atoms at Hartree-Fock (HF), Density-Functional Theory (DFT), and Møller-Plesset (MP2) levels. While in general HF and todays DFT approaches provide often useful results for describing many molecular properties (e.g., NMR data), they fail for the calculation of intermolecular interaction energies, since dispersion-type effects are not or not sufficiently accounted for. However, such interactions are crucial for many chemical and biochemical processes. Here, our new MP2 method for reducing the $O(M^5)$ scaling to linear offers new possibilities, since it allows for the calculation of large systems such as, e.g., an RNA system with 1664 atoms and 19 182 basis functions. We have combined our linear-scaling quantum-chemical methods (QM) also with simple force-field schemes (MM) that allow to describe long-range effects also in systems with more than 1000 or 2000 atoms. It is shown that the convergence with the selected size of the QM region is accelerated as compared to pure QM calculations, however, still large QM spheres are required for reliable descriptions. The presentation will give an overview on new possibilities of quantum-chemical methods for studying in particular intermolecular interactions in complex systems. Examples include intermolecular interactions within molecular recognition processes, RNA-catalyzed Diels-Alder reactions, and cell-receptor virus interactions.

## Conjugated Polymers of the PPE type and their Gold Nanoparticle Complexes

**Uwe Bunz**

*Organisch-Chemisches Institut der Universität Heidelberg, Im Neuenheimer Feld 270, D-69120 Heidelberg*

We describe herein the interaction of negatively charged conjugated polymers of the poly(paraphenyleneethynylene) (PPE) type with gold nanoparticles. The nanoparticles form strong complexes with the PPEs, in which the fluorescence of the PPEs is heavily quenched. Upon addition of a suitable analyte, these complexes are disrupted. The analyte binds to the gold nanoparticle and liberates the PPE, which leads to a fluorescence turn-on. Mathematical analysis of the fluorescence turn-on response allows to discern different biological analytes by their selective fluorescence turn on characteristics.

## Decoding regulatory gene networks – towards a systems biology of development

**Ulrike Gaul**

*Gene Center, LMU Munich, Feodor-Lynen-Str. 25, 81377 Munich*

Biology in general and Developmental Biology in particular are currently experiencing a paradigm shift - from studying individual genes towards analyzing the behavior of entire gene networks. We are interested in understanding the regulation of gene expression and pattern formation, which lie at the heart of animal development, at a systems level. Over the past several years, we have developed a range of experimental and computational methodologies aimed at deciphering the "regulatory code": Where do the cis-regulatory elements lie in the genomic sequence and how do these regulatory elements "compute" expression? In my talk, I will discuss these approaches and present our recent findings on the transcription control of pattern formation in the early *Drosophila* embryo.

## Basic mechanism of myosin motors studied at the single molecule level

**Claudia Veigel**

*Department of Cellular Physiology, Ludwig Maximilians Universität München*

Motor proteins of the myosin family are driving many types of cellular motility. Functions are highly diverse, ranging from muscle contraction to endocytosis, cell locomotion, intracellular transport or signal transduction in the sensory system of the inner ear. Recent structural, kinetic and specifically single molecule studies revealed basic mechanisms of chemo-mechanical energy transduction that are shared amongst the diverse family of myosin motors. This includes mechanisms involved in the production of force and movement, such as conformational changes of the motor coupled to transitions in the biochemical cycle. Other details of the basic mechanism, in particular regulation of motor activity in the cell, however remain unclear. This includes the effect of forces on the mechanics of motor heads and ensembles of motors. We will report on our single molecule mechanical studies using optical tweezers on a variety of myosin motors and discuss implications of these findings for different modes of cellular movement.

Supported by DFG, MRC, NIH and the Royal Society.

## Optical manipulation of gold nanoparticles: from basics to applications

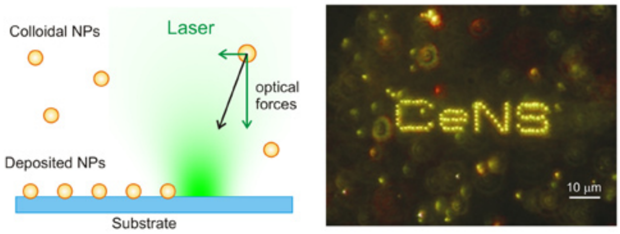
**Andrey A. Lutich**

*Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität München*

A revolution has happened in the last four decades in our understanding of the light-matter interaction. It has given rise to a number of novel research areas and has posed new challenges to the scientific community. The one of the most intriguing is the manipulation of matter by light. By now the optical control has been achieved over a great variety of material systems spanning from individual atoms to entire living cells. This talk will focus on optical manipulation of single Au nanoparticles (NPs). Manipulating individual metal NPs is of exceptional interest because of their unique plasmonic properties that have found a wide range of applications in physics, biology and medicine.

The origin of optical forces acting on a NP exposed to a tightly focused laser beam will be discussed and different approaches to optical manipulation will be defined. We will show how three-dimensional optical trapping of Au NPs is realized in practice and how optical spectroscopy and imaging of trapped NPs is performed by the dark-field microscopy.

A single Au NP optical gun, capable to shoot individual Au colloidal nanoparticles in a desired direction, will be introduced and demonstrated in action. The shooting technique relies fully on optical forces, acting on a gold NP exposed to a single focused laser beam. Optical forces capture the NPs from the colloidal suspension, guide them towards the target position and, finally, immobilize the NPs on a surface. Finally, a single beam optical injection of Au NPs in giant phospholipid vesicles will be shown.



Optical single nanoparticle gun. Left: Sketch of the NP deposition process by the optical gun. Right: A dark-field image of an arbitrary pattern made by deposition single Au NPs. Each bright green spot within the "CeNS" pattern is a single Au NP. Bright spots around the pattern are individual NPs freely floating in the colloidal suspension.

## Quantum dots in photonic crystals: from cavity QED to optical switches and quantum gates

**Jelena Vuckovic**

*Ginzton Laboratory, Stanford University, Stanford, CA, USA*

Quantum dots in photonic crystals are interesting both as a testbed for fundamental cavity quantum electrodynamics (QED) experiments, as well as a platform for quantum and classical information processing. In addition to providing a scalable, on-chip, semiconductor platform, this system also enables very large dipole-field interaction strengths, as a result of the field localization inside of sub-cubic wavelength volumes (vacuum Rabi frequency is in the range of 10s of GHz).

We have probed a strongly coupled quantum dot-cavity system coherently [1], and have demonstrated effects including photon blockade and photon induced tunneling [2] , as well as controlled amplitude and phase modulation between two optical beams at a single photon level [3]. We have also performed resonant spectroscopy of the quantum dot strongly coupled to a cavity [4]. Finally, we have demonstrated fast electrical control of a single quantum dot strongly coupled to a nanocavity [5].

These demonstrations lie at the core of a number of proposals for quantum information processing, and could also be employed to build novel devices, such as optical gates operating at a single photon level and electro-optic modulators and switches with superior performance relative to state of the art devices. For example, fast electrical control of the quantum dot strongly coupled to cavity is important for switching and routing in quantum networks, but can also be employed in an electro-optic modulator controlled with sub-fJ energies (3 orders of magnitude smaller than state of the art devices, while preserving the modulation speed exceeding 10's of GHz).

*[1] Nature, vol. 450, No. 7171, pp. 857-861 (2007)*
*[2] Nature Physics, Vol. 4, pp. 859 - 863 (2008)*
*[3] Science, vol. 320, number 5877, pp. 769-772 ( 2008)*
*[4] Physical Review Letters, Vol 104, 073904 (2010)*
*[5] Physical Review Letters, vol. 104, 047402 (2010)*

## Relaxation dynamics in finite closed quantum systems

**Ulrich Schollwöck**

*Theoretical Nanophysics, Department für Physik, LMU München*

Relaxation and equilibration are usually understood in the framework of a (weak) coupling of the physical system to external degrees of freedom (a bath), which often remains a bit mysterious. But what happens in a strongly interacting, small (a few 100 particles) closed quantum system that has essentially no outside coupling? In this presentation, I want to outline how such a question can be attacked numerically, and then use the methods presented to analyze a problem of far-from equilibrium relaxation that can be implemented experimentally in the framework of ultracold atom gases in optical lattices. I will show how both experimentally (Bloch, Trotzky) and theoretically relaxation occurs, accompanied by the build-up of non-trivial quantum fluctuations: while the system globally never relaxes to an equilibrium ensemble state, each of its subsystems does, while the environment is presented by the remainder of the system.

## Principles of self assembly, from hydrophobic collapse to virus capsid assembly

**David Chandler**

*Department of Chemistry, University of California, Berkeley, Berkeley, California 94720, U.S.A.*

Hydrophobic forces - the forces that cause oil and water to de-mix - often play significant roles in both the thermodynamics and the kinetics of nano-scale self-assembly. This lecture describes principles that underlie these forces, and competition between these forces and geometrical constraints. The competition leads to specific assembled structures. Sometimes, the competition makes kinetics more dominant than thermodynamics.

## Materials in the Flatland

**Kostya S. Novoselov**

*School of Physics & Astronomy, University of Manchester, Oxford Road, M13 9PL, Manchester, UK*

When one writes by a pencil, thin flakes of graphite are left on a surface. Some of them are only one angstrom thick and can be viewed as individual atomic planes cleaved away from the bulk. This strictly two dimensional material called graphene was presumed not to exist in the free state and remained undiscovered until the last year. In fact, there exists a whole class of such two-dimensional crystals. The most amazing things about graphene probably is that its electrons move with little scattering over huge (submicron) distances as if they were completely insensitive to the environment only a couple of angstroms away. Moreover, whereas electronic properties of other materials are commonly described by quasiparticles that obey the Schrödinger equation, electron transport in graphene is different: It is governed by the Dirac equation so that charge carriers in graphene mimic relativistic particles with zero rest mass. The very unusual electronic properties of this material as well as the possibility for it's chemical modification make graphene a promising candidate for future electronic applications.

## Optical Meta Materials and Nano Plasmonics

**Xiang Zhang**

*Ernest S. Kuh Endowed Chair Professor and Director, NSF Nano-scale Science and Engineering Center (NSEC)*
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Recent theory predicted a new class of meta structures made of engineered sub wavelength entities - meta "atoms" and "molecules" which enable the unprecedented electromagnetic properties that do not exist in the nature. For example, artificial plasma and artificial magnetism, and super lens that focuses far below the diffraction limit. The metamaterials may have profound impact in wide range of applications such as nano-scale imaging, nanolithography, and integrated nano photonics.

I'll discuss a few experiments that demonstrated these intriguing phenomena. We showed, for the first time, the high frequency magnetic activity at THz generated by artificially structured "meta molecule resonance", as well as the artificial plasma. Our experiment also confirmed the key proposition of super lens theory by using surface plasmon. We indeed observed optical superlensing which breaks down so called diffraction limit. I'll also discuss nano plasmonics for imaging and bio-sensing. The surface plasmon indeed promises an exciting engineering paradigm of "x-ray wavelength at optical frequency".

## Superconducting nano-sensors for THz radiation detection

**Teun Klapwijk**

*Kavli Institute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, 2600 GA Delft, The Netherlands*

Most of the radiation (90%) emitted in the universe is in the THz range of the electromagnetic spectrum. The most successful detection route is based on various kinds of superconducting devices. High resolution spectroscopy can be done with superconducting tunnel devices or hot-electron bolometers. A major challenge is to find ways for multi-pixel arrays to image the emission from certain astronomical objects. The dominant contenders are transition-edge tensors, which have the needed performance but are difficult to multiplex, and superconducting resonators, which are easily multiplexable but not yet sufficiently mature. The superconducting resonators are rapidly developing and find their way also into other fields of nano-science such as mechanical resonators and circuit quantum electrodynamics.

## Graphene as Unique Multitalent – Catalyst, Semiconductor, Nanowire, Protein Template

**Klaus Müllen**

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Research into energy technologies and electronic devices is strongly governed by the available materials. More recently, carbon allotropes and carbon-rich molecules play an increasingly important role as electronic conductors, semiconductors and catalysts and are attractive alternatives to established organic and inorganic materials. The unique physical and chemical properties of the two-dimensional (2D) π-electron system graphene ask for its chemical synthesis.

We introduce a synthetic route to graphenes which is based upon the cyclodehydrogenation ("graphitization") of well-defined dendritic (3D) polyphenylene precursors. This approach is superior to physical methods of graphene formation such as chemical vapour deposition or exfoliation in terms of its (i) size and shape control, (ii) structural perfection, and (iii) processability (solution, melt, and even gas phase).

Columnar superstructures assembled from these nanographene discs serve as charge transport channels in electronic devices. Field-effect transistors (FETs), solar cells, and sensors are described as examples and their exemplary performance is discussed in terms of supramolecular order and interfacing.

Upon pyrolysis in confining geometries or "carbomesophases", the above carbon-rich 2D- and 3D- macromolecules transform into unprecedented carbon materials and their carbon-metal nanocomposites. Exciting applications are shown for battery cells and fuel cells. Further, transparent and conducting window-electrodes are fabricated which can replace ITO.

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## Nanoscale light control

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Nanostructures can exert a huge influence over light fields. They can confine it on a scale that is (much) smaller than the wavelength or slow it down yielding an excellent compromise between delay and bandwidth. The strong interplay between the geometry and the light results in highly structured light fields on the nanoscale.

In this presentation I will highlight our recent progress in the visualization and manipulation of such light fields. Surface plasmons launched from periodic arrays of holes exhibit the Talbot effect. By mapping the vectorial nature of the electric field, we were able to show the existence of polarization singularities at the nanoscale and measure the mode symmetry of Sommerfeld-like plasmonic nanowire modes. Through a tailored near-field probe geometry we managed to 'see' the magnetic field of light.

Further reading:

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## In situ monitoring of catalysis at the nanoscale

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In situ characterization techniques directly relate the physicochemical properties of a catalyst to its catalytic activity, allowing a more rational catalyst design. As a result of the sensitivity and limitations of each spectroscopic approach, several problems are still unaccounted for (e.g. pressure gap, materials gap and phase gap). These shortcomings can be solved by applying new spectroscopic techniques. Our group has introduced fluorescence microscopy as a sensitive tool to monitor chemical reactions inside zeolite crystals; this directly reveals their catalytic activity and allows locating active zones with submicrometer accuracy, single molecule sensitivity and in three dimensions throughout individual catalysts crystal. Furthermore the scope of this technique extended by using specific probes, that target certain regions inside the catalyst particle. This site specific staining allows a 3D visualization of the particles properties [1,2].

### Hetergeneous catalysis at the nanoscale

We have recorded nanoscale reactivity maps of working catalysts under in situ conditions by localizing single fluorescent reaction products. This is the first approach that allows quantification of the reactivity of catalytic nanodomains. Correlation of these fluorescence nanoscopic reactivity measurements with advanced electron microscopy data will help in rational design of improved catalysts for greening chemistry. This new form microscopy tailored for catalysis is coined NASCA [3].

### Intraparticle diffusion limitation in Ti-MCM-41 catalyzed epoxidation

Mass transfer phenomena are known to play a crucial rule in porous heterogeneous catalysts. When intraparticle diffusion is too slow to provide a sufficient flux of reactants to the inner parts of the catalyst particles, substrate depletion occurs and only the outer parts of the particles are efficiently used for catalysis. Quantifying the degree of intraparticle diffusion limitation by means of the Thiele modulus and the related effectiveness factor remains a big challenge. Only few techniques have the necessary spatial resolution and sensitivity to measure in situ the concentration profiles of products and/or reagents inside the catalytic particles. In this contribution it will be shown how fluorescence microscopy can be used to tackle this problem. The epoxidation of bulky substrates over mesoporous Ti-MCM-41 was chosen as a model case. It is shown how individual reaction events inside the Ti-MCM-41 particles are visualized and localized and how the obtained reactivity maps yield direct information on the Thiele modulus and effectiveness factor of this specific intraparticle diffusion limited catalytic process. Moreover, a value for the intraparticle diffusion constant and the intrinsic rate constant of the catalytic reaction could be estimated based on the data obtained by one in situ experiment. The presented method is versatile and applicable to a variety of catalytic systems, provided that a suitable fluorogenic probe molecule is used, which preferably is detectable at the single molecule level after catalytic conversion [4].

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## Quantum theory of measurement at work by photon counting in a box

**Michel Brune**

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We perform quantum nondemolition (QND) photon counting in a high Q superconducting cavitycavity. Microwave photons are stored for time as long as 0.1s. By using Rydberg atoms as clocks whose ticking rate is affected by the cavity field, we realize an ideal projective measurement of the photon number. The experiment demonstrates all features of quantum measurement theory: random results, state projection and repeatabily. Measuring the atoms is an efficient way for preparing by projection non-classical states such as number states or Schrödinger cat states. We use the QND measurement method for reconstructing the Wigner function of these states and to monitor their decoherence. These field manipulation methods can be extended to state preparation by quantum feedback and to demonstrate non-locality with two fields located in separated cavities.

## Dirac Fermions in HgTe Quantum Wells

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Narrow gap HgTe quantum wells exhibit a band structure with linear dispersion at low energies and thus are very suitable to study the physics of the Dirac Hamiltonian in a solid state system. In comparison with graphene, they boast higher mobilities and, moreover, by changing the well width one can tune the effective Dirac massfrom positive, through zero, to negative.

Negative Dirac mass HgTe quantum wells are 2-dimensional topological insulators and, as a result, exhibit the quantum spin Hall effect. In this novel quantum state of matter, a pair of spin-polarized helical edge channels develops when the bulk of the material is insulating, leading to a quantized conductance. I will present transport data provide very direct evidence for the existence of this third quantum Hall effect: when the bulk of the material is insulating, we observe a quantized electrical conductance.

Apart from the conductance quantization, there are some further aspects of the quantum spin Hall state that warrant experimental investigation. Using non-local transport measurements, we can show that the charge transport occurs through edge channels - similar to the situation in the quantum Hall effect. However, due to the helical character of the quantum spin Hall edge channels, inhomogeneities in the potential profile of the experimental devices have a much stronger effect on the transport properties.

Moreover, the quantum spin Hall edge channels are spin polarized. We can prove this fact in split gate devices that are partially in the insulting and partly in the metallic regime, making use of the occurrence of the metallic spin Hall effect to convert the magnetic spin signal into an electrical one.

Finally, I will address another aspect of Dirac Fermion physics: HgTe of a critical thickness (some 6.3 nm) are zero gap systems and exhibit transport physics that is very similar to that recently observed in graphene.

However, zero gap HgTE wells have a higher mobility than graphene, and also do not suffer from the prsence of more than one valley. This makes them especially suitable to study quantum interference effects under a Dirac Hamiltonian.

# Short Presentations

## Session I

## Session II

# POSTER ABSTRACTS

## SESSION I

# SESSION II

## Mechanical properties of GaAs Micro- and NanoPillars

**Philipp Paulitschke, Norbert Seltner, Heribert Lorenz, Jörg Kotthaus, Eva Weig**

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We investigate the mechanical properties of micro- and nanopillars fabricated from single crystal GaAs by electron beam lithography followed by RIE-etching (Fig1a). The pillars are excited via a shear piezo transducer. They are investigated in an optical setup as well as in the SEM (Fig1b). The aspect ratio of the pillars is varied so that their eigenfrequencies of the transverse fundamental mode range between 100 kHz and 30 MHz. The mechanical properties are investigated as a function of several environments variables such as pressure. The quality factors observed in vacuum are of the order of 1000.

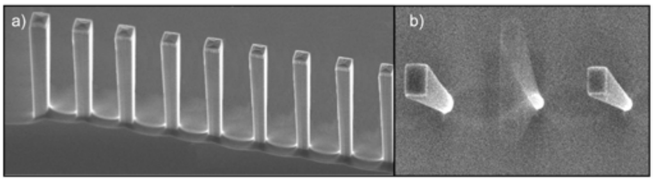

Fig1. SEM picture of GaAs pillars a) with a gradient in the radius and b) oscillating pillar at his eigenfrequency.

## Triggering the Volume Phase Transition of Au Nanorod-Microgel Nanocomposites with Light

**Jessica Rodríguez-Fernández, Michael Fedoruk, Calin Hrelescu, Andrey A. Lutich and Jochen Feldmann**

*Photonics and Optoelectronics Group and CeNS, Physics Department, Ludwig-Maximilians-Universität München, Germany*

Hybrid nanocomposites offer the unique advantage to integrate the multifunctionality provided by two or more building blocks on a very small scale. Of special interest in the field is the possibility to tune the response of those hybrids in a remote and controlled way by exploiting the external tunability provided by one of the components. In this work we have prepared hybrid nanocomposites based on the combination of Au nanorods (NRs) and thermoresponsive (pNIPAM) microgels with a core-shell type geometry [1]. We demonstrate that in this type of nanocomposites a fast and remote control over the volume phase transition (deswelling) of the encapsulating pNIPAM can be achieved by using the Au NR cores as light-triggered nanoscale heating sources. We prove the light-driven tunability of our nanocomposites by measuring *in situ* the changes in the optical response of the encapsulated Au NRs while irradiating them with a NIR laser, which also allowed us to prove the reversibility of this light-driven tuning. Our results highlight the potential of this type of nanostructures as remotely-controlled optomechanical actuators, which may find application in fields such as drug delivery or nanoscale motion.

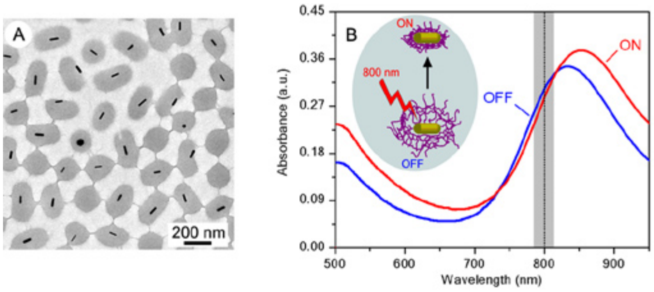

Fig.1 (A) Representative TEM micrograph of pNIPAM-encapsulated Au nanorods. (B) vis-NIR extinction spectra of the Au NR@pNIPAM nanocomposites before (blue line) and during (red line) irradiation with a cw laser ($\lambda$=800 nm, 880 kW/$\text{cm}_2$). The vertical dashed line indicates the operating laser wavelength and the shaded area, the spectral range of the notch filter used. The inset illustrates the induced collapse of the pNIPAM shell due to the optothermal heating of the Au NRs during irradiation with a NIR laser.

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## Linking Organic Molecules to Silicon Oxide Surfaces: a Simplified Coupling Chemistry

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We have investigated the pH-dependent linkage of carboxymethylated amylose to organosilanized surfaces using AFM based single-molecule force spectroscopy. As expected, at pH 7.4 activation of the carboxylic acid with EDC/NHS is required to form a stable link between the AFM tip and the substrate surface. In this case an amide bond can be formed between a carboxyl group of CMA and an amino group of the DETA-functionalized surface. At pH 2.0 we found that no activation of the carboxylic acid is required for bond formation. In this case the mean bond rupture force decreases and at the same time the coupling efficiency increases, compared to experiments at pH 7.4. The difference in bond rupture forces indicates that at pH 7.4 with EDC/NHS and at pH 2.0 without EDC/NHS, the scission of two different bonds is observed. The systematic variation of the organosilane functionalization of AFM tip and substrate surface showed that coupling at pH 2.0 without EDC/NHS requires free silanol groups on the surface. Amino groups most likely do not contribute to coupling at low pH. The most likely scenario for bond formation at pH 2.0 is acid-catalyzed ester condensation between a carboxyl group of CMA and a free silanol group in the surface anchor or on the silicon surface. This can be used as a simple and efficient strategy for linking organic molecules to silicon or silane functionalized inorganic surfaces.

## PcrA helicase dismantles RecA filaments by reeling in DNA in uniform steps

**Jeehae Park, Sua Myong, Anita Niedziela-Majka, Kyung Suk Lee, Jin Yu, Timothy M. Lohman, Taekjip Ha**
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Translocation of helicase-like proteins on nucleic acids underlies key cellular functions. However, it is still unclear how translocation can drive removal of DNA bound proteins, and basic properties like the elementary step size remain controversial. Using single molecule fluorescence analysis on a prototypical superfamily 1 helicase, *Bacillus stearothermophilus* PcrA, we discovered that PcrA preferentially translocates on the DNA lagging strand instead of unwinding the template duplex. PcrA anchors itself to the template duplex using the 2B subdomain and reels in the lagging strand, extruding a single stranded loop. Static disorder limited previous ensemble studies of PcrA stepping mechanism. Here, highly repetitive looping revealed that PcrA translocates in uniform steps of 1 nt. This reeling-in activity requires the open conformation of PcrA and can rapidly dismantle a preformed RecA filament even at low PcrA concentrations suggesting a mode of action for eliminating potentially deleterious recombination intermediates.

## Accelerating fluorescence resonance energy transfer with plasmonic nanoresonators

**Frank Jäckel, V. Faessler, C. Hrelescu, A. A. Lutich, L. Osinkina, S. Mayilo#, J. Feldmann**
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Fluorescence resonance energy transfer (FRET) is at the heart of light harvesting in photosynthetic systems and of many applications including single-molecule spectroscopy and organic electronic devices. Control of FRET-efficiencies and rates can therefore be beneficiary to these applications. A large variety of plasmonic nanostructures has been shown to greatly enhance and modify optical processes due to their localized surface plasmon resonances [1,2]. When excited at resonance they give rise to strongly enhanced and highly localized electromagnetic fields. In particular, plasmonic nanoresonators, i.e., pairs of two noble metal nanoparticles separated by less than the particle radius, have been shown to greatly enhance Raman scattering [3] and fluorescence [4,5].

Here, we show for the first time that FRET can be accelerated by plasmonic nanoresonators and that the nanoresonators enhance FRET more efficiently than isolated particles [6]. We further present model calculations that compare FRET rates in nanoresonators and individual particles and that support the superiority of nanoresonators for FRET-enhancement.

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## Anomalous transport of proteins bound to a crowded membrane

**Thomas Franosch[1,2,3], F. Höfling[4,5], T. Bauer[2,3], E. Frey[2,3], M. R. Horton[3], J. O Rädler[3]**
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Cell membranes consist of a a heterogeneous lipid bilayer, densely packed with integral and peripheral proteins. Proteins confined or bound to such membranes explore a quasi-two-dimensional, highly crowded and heterogeneous landscape. Their motion displays slow diffusion and anomalous transport [1]. A similar phenomenology is provided by a two-dimensional Lorentz model, where a Brownian tracer diffuses between randomly distributed discs. Extensive computer simulations show that at a certain critical obstacle density, the dynamics becomes subdiffusive over many decades in time, which is attributed to an underlying continuum percolation transition.The model exhibits slow dynamics, anomalous transport, and a localisation transition [2,3,4].

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## Single Basepair Distance Sensitivity Obtained by Protein Induced Fluorescence Enhancement

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Although single molecule FRET allows monitoring of the interaction between a protein and a nucleic acid, it requires fluorescent tagging of the protein and the involved distance range of 25-75 Å range. Using BamHI, RIG-I, and RecA as test systems, we present a systematic characterization of the protein induced fluorescence enhancement technique which circumvents protein labeling and displays a strong distance sensitivity below 34 Å, where FRET is insensitive with the resolution of a single basepair and a single nucleotide of DNA.

## TEM Studies on the Crystallographic structure of E. huxleyi Coccolith plates

**Ramona Hoffmann[1], E. Griesshaber[1], J. Young[2], C. Scheu[3], A. Müller[3], A. Wochnik[3], S. Matich[4], W. W. Schmahl[1]**

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Coccolithophores are single-celled marine algae. They are covered by a shell composed of nanostructured $CaCO_3$ plates, the coccoliths. Coccolithophores contribute roughly 15 % to the oceanic biomass and play important roles in the dimethylsulfide production and the global ocean carbon cycle. There are 280 species, most of which are highly adapted to different habitats. In this work we focus on the species *Emiliana huxleyi* which is the most common coccolithophore and which can tolerate different temperature, light and nutrient conditions.

Based on optical and AFM observations (Young et. al., 2003), the coccoliths are currently assumed to be composed of two single crystalline nanosized elements of complex shape. These so-called R- and V-units are intricately interlocked to form a spoke-wheel-like composite structure. However, most carbonate-based biomaterials (e.g. nacre, brachiopods and mollusc shells) are formed by mesocrystals. Mesocrystals are three-dimensionally ordered aggregates of primary nanoparticles, usually in an organic matrix. Due to the 3-dimensional orientational correlation of the nanoparticles, mesocrystals are frequently not properly distinguishable from “single crystals”.

We employ Transmission Electron Microscopy (TEM) to investigate the nanostructural organisation of the coccolith skeleton. The samples were collected from the South Atlantic Ocean and were prepared on Millipore filters. FIB lamellae were cut out from the coccoliths and were used for TEM imaging and electron diffraction. The diffraction patterns showed mosaic-spread typical for mesocrystals. However, electron beam damage occurred rapidly and the diffraction patterns taken after the TEM observation showed transformation into a disordered polycrystalline structure.

The aim of our further studies is to investigate in great detail the hierarchical structure and chemical signatures of the coccoliths from different species and from distinct marine habitats by using TEM imaging, Electron Energy Loss Spectroscopy (EELS) and Electron Backscattered Diffraction (EBSD).

## Self-assembly of DNA into well-defined structures used as templates and biosensors

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Molecular self-assembly enables the ‘bottom-up’ construction of well-defined structures with nanometer precision. The Watson-Crick complementarity of base pairing offers highly selective binding of DNA strands. The recently established DNA origami method employs this mechanism to create two and three-dimensional DNA objects of arbitrary shapes and patterns [1, 2]. DNA origami objects are built from a virus-based single DNA strand that is folded into shape by hundreds of short oligonucleotides. We here present three projects to illustrate the potential of this versatile enabling technique:

1. A three-dimensional DNA tetrahedron consisting of rigid six-helix bundles is built, where up to 66 selective positions can be addressed by attachment of fluorescently labeled oligonucleotides. High-resolution blink microscopy offers the opportunity to verify the correct folding of the tetrahedron into its designed shape. Such fully addressable three-dimensional templates could be employed as biosensors or as rigid structural elements for nanofabrication.
2. The precise determinability of fluorophore positioning is exploited by creating a planar DNA origami block used as breadboard for fluorescence resonance energy transfer (FRET) measurements. The primary advantages over previous FRET measurements, where an individual DNA helix was used as spacer between donor and acceptor dyes, are the avoidance of side effects caused by the relatively short persistence length of double-stranded DNA and potential fluorescence quenching by bases located between donor and acceptor.
3. Organizing gold nanoparticles (AuNP) precisely on self-assembled DNA origami structures is of great interest for nanophotonics and nanoelectronics applications. AuNP conjugated to a controlled number of DNA single strands are hybridized to designated sites on various DNA origami structures. Following this route, we demonstrate the formation of arbitrary AuNP patterns on DNA origami templates and the metallization of DNA structures using site-directed growth of gold clusters.

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## Device Physics of Nanostructured $TiO_2$-P3HT Hybrid Solar Cells

**Jonas Weickert[1], Claudia Palumbiny[1], Julian Reindl[1], Andreas Wisnet[2], Christina Scheu[2], Lukas Schmidt-Mende[1]**

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Organic solar cells are a promising new technology due to their easy processibility and potential low cost production. Power conversion efficiencies of 5-6% have been reported recently for poly(3-hexylthiophene) (P3HT):fullerene bulk heterojunction solar cells. However, the morphology of the active layer cannot be directly controlled. There are only limited studies on morphological effects on device physics and the "ideal" morphology is still unknown.

The introduction of nanostructured $TiO_2$ is an interesting approach to influence the morphology of the solar cells bulk heterojunction. P3HT can be infiltrated into dye-sensitized $TiO_2$ which also exhibits favorable electronic properties as electron collecting electrode. Additionally, confinement inside the nanostructures can enhance the hole mobility of P3HT. The heterojunction morphology can be directly controlled via shape and structure of the $TiO_2$ and the device absorption tuned by choosing an appropriate dye.

$TiO_2$ nanostructures are fabricated by anodization of Ti thin films or $TiO_2$ electrodeposition onto anodized alumina membranes yielding nanotubes and nanowires, respectively. Device physics are studied using spectrally resolved external and internal quantum efficiency and photoluminescence measurements, time resolved transient experiments and device characterization under varying illumination levels. The influence of the heterojunction morphology on charge separation, recombination and transport is analyzed to infer general design rules for organic and hybrid solar cells.

First results reveal that charge carrier recombination seems to be less enhanced than charge separation for nanostructured devices compared to bilayer solar cells indicating that an ordered interpenetrating donor-acceptor interface is desirable in organic solar cells.

$TiO_2$ nanostructures are further analyzed using high resolution transmission electron microscopy by Andreas Wisnet, Group Prof. Scheu, LMU Munich. Results are presented in the contribution "TEM investigation of nanostructured hybrid solar cells".

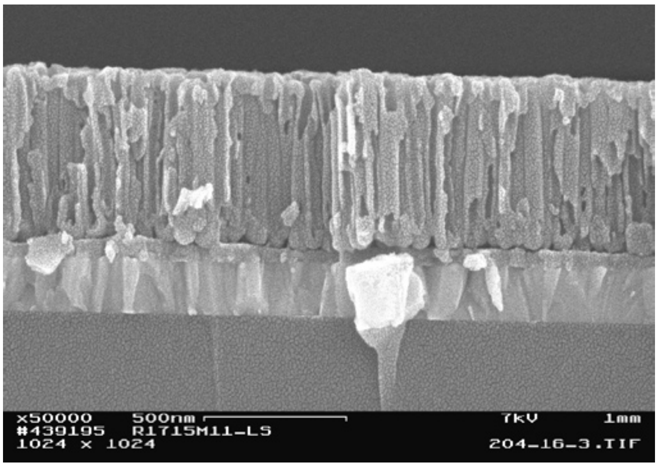


Fig. 1: Scanning electron microscopy side view of typical $TiO_2$ nanotubes from anodization of 400 nm Ti on indium-tin oxide covered glass.

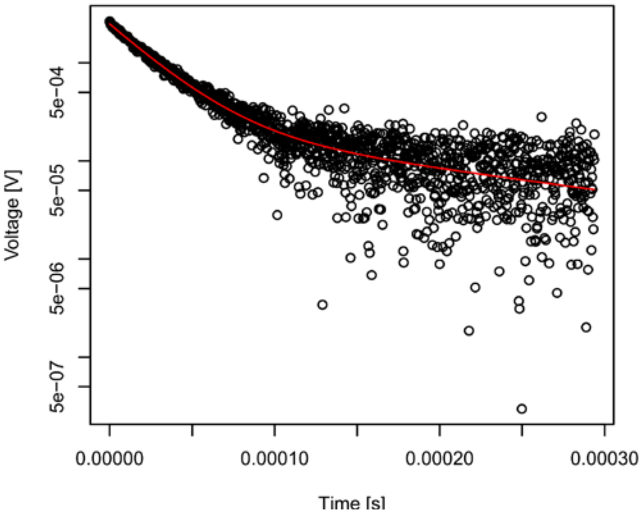


Fig. 2: A typcial transient photovoltage decay.

## EcoRV dynamics in a crowded environment

**Leila Esmaeili Sereshki, Ralf Metzler, Michael Andersen Lomholt**

*Physics Department TU Munich*

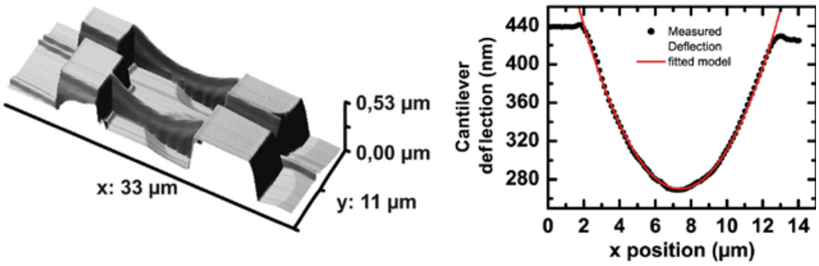
EcoRV is a restriction enzyme that cleaves the DNA on a special sequence and acts as an immune system for E.coli. If a virus attacks the bacterium, EcoRV should find the viral DNA quickly, and cleave it. Recent experimental evidence strongly suggests that larger biopolymers in living biological cells perform anomalous diffusion due to crowding inside the cell. At present, within the framework of "structured view" of cytoplasm among others, based on micrographs it has been suggested that the cytoplasm of a bacteria cell resembles a random fractal structure. Following this view we model the cytoplasm as a random fractal generated by bond percolation to mimic certain features of diffusion under conditions of molecular crowding. In addition, there is a consensus that EcoRV can be found in two configurational states. The unbound protein may oscillate between the structure with a closed cleft, and another state where the cleft is open enough to bind to the native or foreign DNA nonspecifically. Under subdiffusion condition, the presence of a dormant/closed state increases the EcoRV binding rate to a DNA target in the cell. We quantify the search of EcoRV for a target DNA in the cell. We suggest that crowding-induced anomalous diffusion may indeed be beneficial for the cell's regulatory processes, and is in line with an emergent, more local picture of the dynamics of cellular control and defence.

## Investigation of a nanomechanical system with scanning probe microscopy

**Johannes Rieger, E. M. Weig and J. P. Kotthaus**

*Center for Nanoscience and Department of Physics LMU München – Germany*

The atomic force microscope has become an extremely powerful tool for the investigation of nanoscale structures. In addition to providing information about a sample's topography, it allows spatially resolved measurements of certain local properties such as spring constants, magnetization, capacitance, etc. The development of small mechanical elements for this application has ultimately led to the rapidly evolving field of nanomechanics.



Left: Contact mode image of two doubly clamped silicon nitride beams. Right: Cut of the data along the beam in the front of the image to the left. The model of a string under tensile stress yields a quadratic behaviour and was fitted to the data, yielding a tensile stress of 62 MPa.

Here we report on the investigation of the mechanical properties of a doubly clamped silicon nitride beam under high tensile stress by means of atomic force microscopy (we use an Attocube AFMI). From constant force measurements we are able to extract the intrinsic tensile stress of the material in excellent agreement with the value obtained by a measurement of the linear frequency dependant amplitude response of the resonator. In the future, we plan on utilizing the setup to gain access to dynamical properties of the nanomechanical system such as the mode shape of the driven beam or the frequency response of a resonator subject to an additional force exerted by the AFM-cantilever.

## Active enzymes covalently bound to the walls of mesoporous silica films

**Stefan Niedermayer, Andreas Zürner, Axel Schlossbauer, Bastian Rühle, Thomas Bein**

*Department of Chemistry and Center for Nanoscience (CeNS), University of Munich (LMU)*

Based on their high selectivity and activity at moderate temperatures, enzymes are attractive catalysts with numerous industrial applications. One major problem in using enzymes as catalysts arises from their sensitivity towards process parameters such as pH and temperature variations. Such problems can be potentially overcome through incorporation of enzymes into host systems with pore sizes of the same dimension as the enzyme. Additionally, covalent attachment to the host material prevents leakage of the catalyst and results in facile separation from the reaction solution and thus, enhanced reusability.

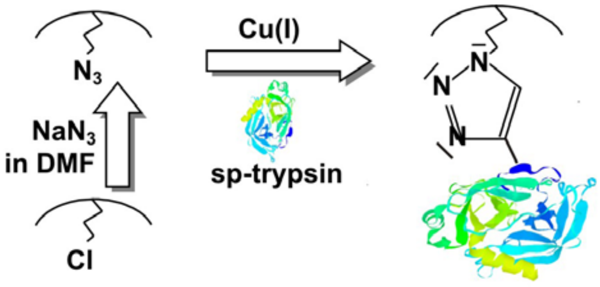


Figure 1: Schematic procedure for covalent bonding of sp-trypsin to the walls of mesoporous silica thin films.

Here we show the covalent binding of trypsin to the pore walls of a mesoporous thin silica film by the use of a copper(I)-catalyzed Huisgen 1,3-dipolar cycloaddition of alkyne and azide functionalities. We prepared thin mesoporous films templated with the surfactant Pluronic F127 to ensure pores that are larger than the diameter of trypsin. During extraction of the template with ethanol, a shrinkage of the film in z-direction of ~30% could be observed, resulting in elliptical pores. Afterwards, the pore walls were modified with 3-(chloropropyl)triethoxysilane followed by azide exchange to create anchor groups for sp-modified trypsin molecules as shown in Figure 1.

To investigate enzyme activity, two different kinds of film samples were prepared. One sample was prepared with F127 and another without template, which results in a dense silica film. Activity was investigated using the enzymatic digestion of 4-methylumbelliferyl 4-guanidinobenzoate hydrochloride to 4-methylumbelliferone, which can be monitored via its fluorescence. These experiments showed a much higher activity of enzyme-containing mesoporous silica films compared to dense silica films, thus confirming that enzyme molecules have been anchored inside the pores of the film. We will discuss the impact of different mesoporous silica host structures on the catalytic activity of the enzyme-containing thin films.

Acknowledgement: The authors are grateful for funding from DFG through the SFB 749 and the NIM cluster.

## Transmission electron microscopy study on domain formation and critical thickness of ferroelectric lead titanate thin films

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$PbTiO_3$ films with various thicknesses were epitaxially grown by RHEED assisted pulsed-laser deposition on (001)-$SrTiO_3$ and (110)-$DyScO_3$ substrates. We used high-resolution transmission electron microscopy to investigate the (90°) domain structure in the films. They contain predominantly c-domains with a minor fraction of a-domains that is clearly higher in case of $DyScO_3$ than $SrTiO_3$. In $PbTiO_3$ on $SrTiO_3$ the a-domains have wedge shape, whereas in $PbTiO_3$ on $SrRuO_3/DyScO_3$ they have nearly uniform width. Detailed analyses show that the domain walls contain (100) and (001)-oriented steps. These steps are clearly more abundant in case of $SrTiO_3$ than of $SrRuO_3/DyScO_3$ and are responsible for the observed wedge shape. The observed difference in a-domain shape induced by the two substrates is attributed to a higher stiffness of $SrTiO_3$ than of $SrRuO3/DyScO_3$ as we corroborated with nanoindentation experiments.

In another set of experiments we have grown $PbTiO_3$ film with 'a' domains and also completely c-oriented $PbTiO_3$ films of various thicknesses (22-350 nm) on $SrTiO_3$. The influence of laser pulse frequency, substrate termination on growth and functional properties were studied using transmission electron microscopy, atomic force microscopy, and Xray diffraction. The $PbTiO_3$ films were grown with changing parameters like laser pulse frequency (growth rate), cooling rate, oxygen-partial pressure and substrate (termination) treatment. At low laser pulse frequencies (≤ 5 Hz) a-domains did not develop up to large thickness (larger than 250-340 nm) independent of the quality of the substrate treatment (i.e. fraction of $TiO_2$ termination), oxygen partial pressure and cooling rate. At high laser pulse frequencies (≥8 Hz) a-domains develop above critical thickness (typically between 20-100 nm) even for perfect 100% $TiO_2$ terminated substrates. In these cases secondary phase were generally detected (XRD/TEM) which are expected to act as nucleation sites for a-domain formation. Our thick mono-domain strained $PbTiO_3$ films exhibit huge increase in $T_c$ from the bulk value of 492°C to 840°C. PFM results shows that the films were ferroelectric in nature.

Further nanoscale structural and chemical investigations of superlattice thinfilms of ferroelectric and multiferroics using different characterizing methods of TEM is in progress at the group of Prof. Scheu.

## Non-linear Photoluminescence from pristine Graphene

**Matthias Handloser**[a], **Giovanni Piredda**[a], **Antonio Lombardo**[b], **Andrea C. Ferrari**[b], **Achim Hartschuh**[a]

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Graphene is in the focus of research due to its unique electronic and optical properties. Intrinsic graphene is a zero gap semiconductor with a linear dispersion relation for E-k leading to zero-effective-mass electrons and holes described by Fermi-Dirac theory. Since graphene has no bandgap no photoluminescence would be expected. However, recently two groups showed non-linear photoluminescence from pristine graphene putting forward two different physical models explaining this remarkable effect [1,2].

We performed a detailed spectroscopic investigation varying both excitation energies and intensities to test these models. Graphene photoluminescence is found to be very broad ranging from 600 to 1200 nm. While we observe different photoluminescence spectra at different excitation energies no pronounced power dependence is found.

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*[2] R.J. Stöhr, R. Kolesov, J. Pflaum and J. Wrachtrup "Fluorescence of laser created electron-hole plasma in graphene"arXiv:1006.5434v1 [cond-mat.mtrl-sci] 2010*

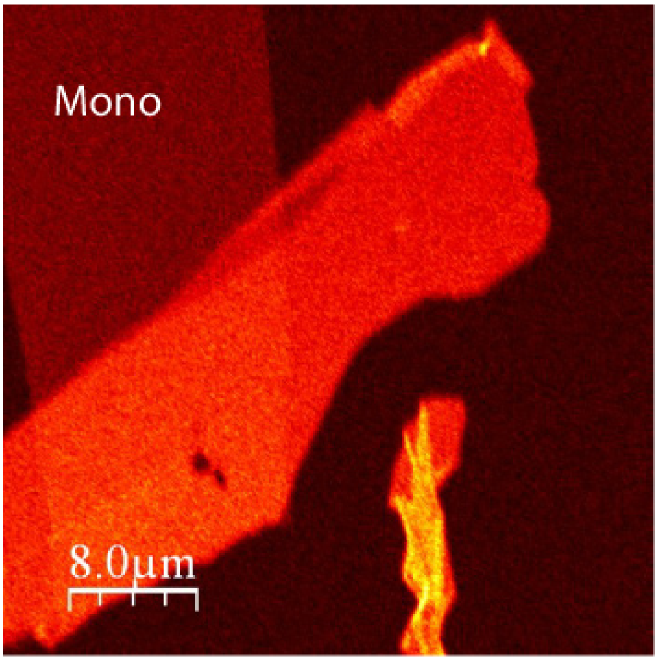

Figure: Photoluminescence from mono- and multi-layer graphene on glass detected between 863-1000 nm after femtosecond laser excitation at 800 nm.

## Optical spectroscopy at sub-Kelvin temperatures

**Felix M. Mendoza, E. Schubert, F. Donhöfner, S. Ludwig and A. Högele**

*CeNS and Fakultät für Physik, Ludwig-Maximilians Universität München*

Over the past decades transport phenomena in mesoscopic structures have exhibited rich physics. The quantum point contact in particular, has been extensively studied and shows conductance quantization at low temperatures. Its conductance increases in integer steps of conductance quanta, but also exhibits an additional conductance feature at 0.7 quanta, the so-called 0.7-anomaly. To date, the origin of this 0.7-anomaly is still subject to controversy. Recent theory suggests that the anomaly is associated with increased spin fluctuations in the quantum point contact. To study spin physics in quantum point contact structures, or in any other generic mesoscopic system, we propose an all-optical spectroscopy technique based on the magneto-optical Faraday or Kerr effect. To this end, we are developing an optical microscope for measurements at sub-Kelvin temperatures in a He-3 system. It will combine diffraction-limited spatial resolution and nanometre precision positioning of the sample, which, in combination with Faraday or Kerr rotation signal, will enable spatial imaging of local spin textures and shed new light on old physics problems in mesoscopic systems.

## Signatures of Anderson Orthogonality in absorption spectra

**Wolfgang Münder, A. Weichselbaum, and J. von Delft**

*CeNS and Fakultät für Physik, Ludwig-Maximilians Universität München*

Since the late 1960's it is known that the response of a Fermi sea to changes in a local scattering potential results in a change of the scattering phase shifts of all the single-particle wave functions, which is known as Anderson Orthogonality [1]. This causes the ground states of the system before and after the change to be orthogonal in the thermodynamic limit. Moreover, it is also known that Anderson Orthogonality also influences dynamical properties of the system like optical absorption spectra, which has been shown analytically at that time for the X-Ray edge effect [2,3,4,5]. In recent work this has been extended to the context of the Kondo exciton [6,7]. In this work, we establish a formalism to study signatures of the Anderson Orthogonality in optical absorption spectra in the general case of a switch between an initial Hamiltonian and a final Hamiltonian. Based on this, we study the Anderson Orthogonality for a series of models of increasing complexity within the framework of the numerical renormalization group, NRG [8].

*[1] P. W. Anderson, Phys. Rev. Lett. 18, 1049 (1967)*
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*[3] J. J. Hopfield, Comments Solid State Phys. II, 2 (1969)*
*[4] G. D. Mahan, Phys. Rev. 163, 612 (1967)*
*[5] B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. 178, 1072 (1969); P. Nozières, J. Gavoret, and B. Roulet, Phys. Rev. 178, 1084 (1969); P. Nozières, and C. T. De Dominics, Phys. Rev. 178, 1097 (1969)*
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*[8] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975)*

## Inorganic-Organic Core-Shell Nanoparticles – PEGylated Colloidal Mesoporous Silica

**Christian Argyo, Valentina Cauda and Thomas Bein**

*Department of Chemistry and Center for Nano Science (CeNS), University of Munich (LMU)*

Colloidal mesoporous silica (CMS) nanoparticles have been proposed as promising drug delivery systems for cancer cell targeting. In particular, inorganic-organic core-shell nanoparticles have received great attention since they can offer encapsulation of molecules in the mesopores, stimuli-responsive controlled release, and selective affinity to biological tissues.

Grafting of the hydrophilic polymer poly(ethylene glycol) (PEG) onto the surface of inorganic particles can provide an effective improvement of the surface properties by preventing particle aggregation and inducing a stabilization of the colloidal suspension. Mesoporous silica as a core of such hybrid particles features several superior properties, such as the possibility of tailoring the internal pore functionalization, the pore size and the pore volume, respectively.

We have synthesized CMS nanoparticles with a selectively functionalized linear-PEG shell on the outer surface, prepared by a delayed co-condensation approach with a PEG-trialkoxy silane precursor. A second approach is based on a surface-initiated light-induced free radical polymerization on externally vinyl-functionalized CMS nanoparticles, thus obtaining for the first time a shell of branched PEG chains on such systems.

Characterization with several techniques shows the successful preparation of inorganic-organic core-shell nanoparticles. Both linear and branched PEGylated CMS nanoparticles feature high colloidal stability in aqueous solution, high surface area and pore volume. The behavior of linear PEG-coated CMS nanoparticles was investigated in simulated body fluid (SBF), with the aim of gaining new insights regarding the stability and biodegradability. Depending on the density of the coverage and the chain length of the polymer, the PEG-shell reduces the rate of biodegradation of silica in simulated body fluid. The present studies extend the PEGylation approach to develop biocompatible hybrid nanocarriers for drug delivery applications.

Acknowledgement: The authors are grateful for funding from the DFG through the SFB 749.

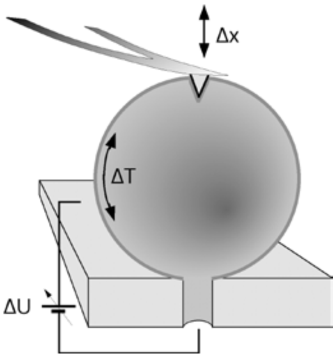
## Cell membrane in tension

**Stefan Scheuer, Hubert Krammer, Evren Pamir, Martin Benoit and Niels Fertig***
*LS Gaub, CeNS, LMU-München, Amalienstr. 54, D-80799 München, Germany*
**Nanion Technologies GmbH, Erzgiessereistr. 4, D-80335 München, Germany*

Cell membranes separate the extracellular world from the intracellular space. This border made from a lipid bi-layer contains proteins for various tasks (ion transport, sensors, specific adhesion... ). They interact and communicate with the extracellular world.

Adhesion for example can promote anchorage, motion, communication, food intake and even more. The membrane is very flexible and deformable and easily can adapt to the structure of the surface it wants to adhere to. By AFM force measurements we found molecular adhesion forces ranging between a few up to some tens of pico Newtons. In a combined patch-clamp AFM setup, we simultaneously monitor an applied trans-membrane voltage, trans-membrane ion currents and membrane movement. With this setup simultaneously a variety of membrane parameters such as membrane tension (T), membrane capacitance, electrical fields or ion currents become accessible. Here we present Prestin as an example of a voltage dependent membrane motor protein.

Still there is little known about the function of Prestin. In this investigation on a patch-clamped cell we characterized the mechanical membrane motion (Δx) in the order of a few nano Meters induced by an electrical stimulation (ΔU) of some milli Volts.



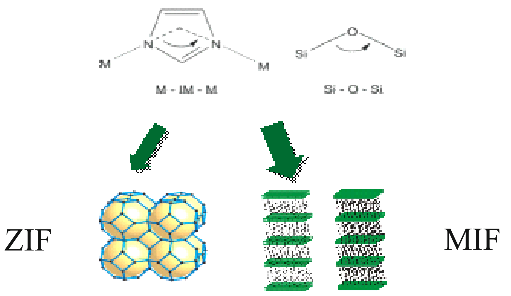
## Mesostructured metal organic frameworks (MIFs)

**Sebastian C. Junggeburth,* Kulpreet Virdi, Christina Scheu, und Bettina V. Lotsch**
*Department Chemie und Biochemie, Lehrstuhl für Anorganische Festkörperchemie, Ludwig-Maximilians-Universität München*

Recently we discovered a new class of mesostructured metal-organic frameworks, christened mesostructured imidazolate frameworks (MIFs), by a surfactant-assisted synthesis approach.

The synthesis affords templated mesostructures, which are thermally stable up to 300 °C and show the XRD signature of lamellar materials. Due to similar bridging angles Zn-Im-Zn (Im = Imidazolate) and Si-O-Si, a topological relationship between templated zinc imidazolates and mesoporous silicates is inferred by anaolgy to the known mesoporous MCM-type phases (see Figure).

[1] K. Park, Z. Ni, A. P. Côté, J. Y. Choi, R. Huang, F. J. Uribe-Romo, H. K. Chae, M. O'Keeffe, O. M. Yaghi, PNAS, 2006, 103, 10186.



Scheme 1. The bridging angles in metal IMs and zeolites.

By choosing the right conditions our mesostructured MIF can be transformed to the microporous ZIF [1].

## Covalent coupling of organic molecules via dehalogenation and addition reactions on Au(111)

**Stefan Schlögl, Hermann Walch and Markus Lackinger**
*AG Lackinger, Geowissenschaftliches Institut, Sektion Kristallographie, LMU München*

In order to tailor mechanical, chemical, and electronic properties of two-dimensional materials and eventually devices, a bottom-up surface mediated fabrication process under controlled conditions seems promising. The halogenated compound 1,3,5-triiodobenzene (TIB) was chosen as monomer for a two step synthesis of aromatic porous two-dimensional (2D) Covalent Organic Frameworks (COF). The compound was preheated to ~ 400 K in vacuum to facilitate sufficient vapour pressure, and then deposited through a leak valve onto Au(111) held at room temperature under ultrahigh-vacuum conditions. Upon adsorption, all three C-I bonds of TIB monomers were cleaved, leaving chemisorbed iodine and phenyl radicals on the surface. Iodine is known to form chemically stable bonds with gold atoms, which in the present case yields extended one-atom-high hexagonal iodine domains. The coverage was close to one monolayer per unity, and the experimental lattice parameter of 0.55 nm is in accordance with literature values. Remaining phenyl triradicals were found located close to step-edges and interconnected by covalent C-C bonds to porous networks with a spacing of 0.74 nm between adjacent pores. Those dimensions are in excellent agreement with DFT calculations of a 2D polymer based on symmetrically triply σ-σ interlinked phenyl rings.

Thermal annealing of as prepared samples to ~670 K resulted in desorption of most iodine atoms, while the 2D phenyl derived domains remained stable and their domain size increased.

## Quality Factors of Nanomechanical Resonators

**Thomas Faust**, **Quirin Unterreithmeier and Jörg P. Kotthaus**
*Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany*

The study of nanomechanical resonant motion is a rapidly advancing field of science with prospects in fundamental studies and applications. For many aspects, a low mechanical friction (or high quality factor) is advantageous. It has been experimentally shown that silicon nitride resonators under high uniform tensile stress exhibit significantly higher quality factors than unstressed ones of the same resonance frequency. The underlying mechanism, however, is yet to be known.

Measuring the room-temperature quality factors of the fundamental and higher harmonic modes of our high stress SiN nanomechanical oscillators with cross sections of 200x100 nm and lengths ranging from 35 to 5 micrometer, we find a strong mode dependence of the quality factor [1]. This can be explained by applying a damping model based on continuum mechanics.

Assuming the friction throughout volume of the resonator to be caused by the local strain variations as the beam oscillates, we are able to quantitatively model the observed quality factors introducing a frequency-independent imaginary part of the Youngs modulus [Fig. 1]. Based on our calculations we can deduce that the high mechanical quality factors are caused by the increase in elastic energy rather than a decrease in energy loss with increasing tensile stress. Therefore, we expect that resonators consisting of nearly any material will exhibit higher quality factors when stressed.

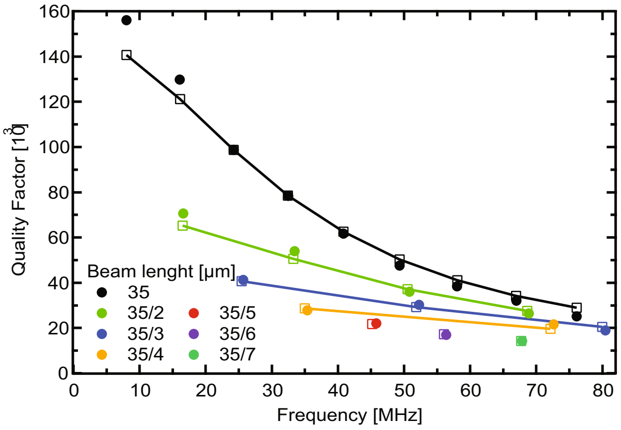


Fig. 1: Frequency and mechanical quality factors of the measured resonances (solid dots); the lengths of the beams are colour-coded. The hollow squares represents our modelling of the resonance frequencies as well as the quality factors. As a guide to the eye, the various harmonics corresponding to the same beam are connected.

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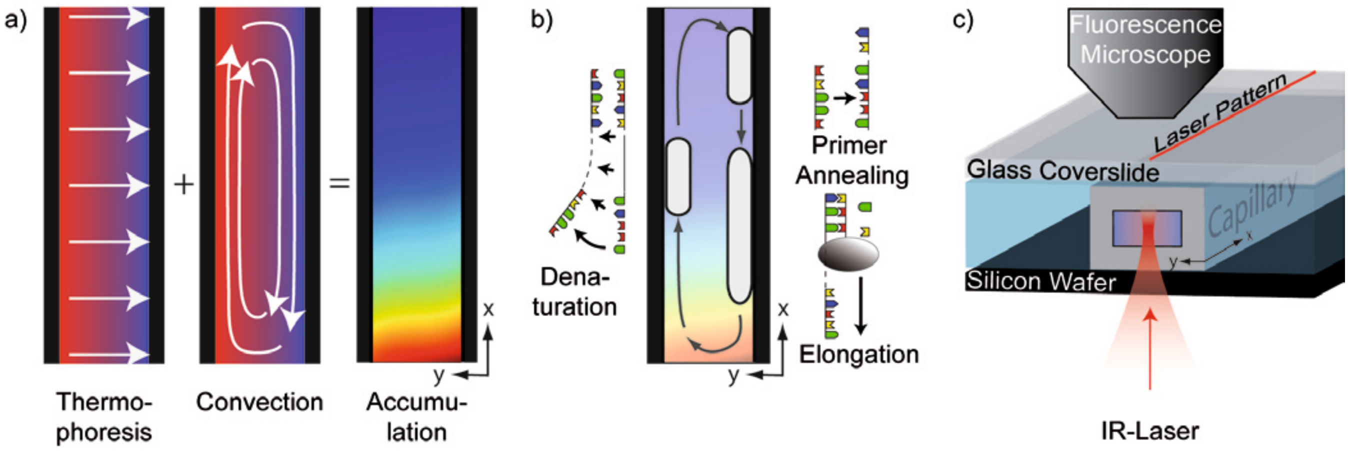
## A Thermal Trap for DNA Replication

**Christof B. Mast**, **Dieter Braun**
*Fakultät für Physik and Center for NanoScience (CeNS), Ludwig-Maximilians-Universität München, Germany*

Normally, genetic information is protected from free diffusion into the environment by cell walls. The cells provide all conditions for the replication and mutation of genetic material - the basic prerequisite for Darwinian evolution. We modeled a fundamental principle in the laboratory, which allows for continuous evolution of genetic material without cell membranes. We filled a thin capillary with DNA and nucleotides, solved in buffer as an aqueous solution (Figure c). A moving infrared laser spot then generated a thermal gradient realizing thermophoresis as well as a cyclic convection of the solution. The superposition of both effects caused the double-stranded DNA molecules to migrate to the cold area (Figure a), while simultaneously cycling the DNA between the cold and warm section of the capillary. In the hot area, the DNA separates into single strands. These are then elongated by a polymerase enzyme in the cold region to two double-stranded copies of the original template DNA (Figure b). Therefore, a simple temperature gradient drives both, an exponential replication as well as the selective accumulation of information. This is relevant as presumably similar thermal conditions prevailed in rock pores near hot undersea springs of prehistoric oceans. Our experiment shows how a simple disequilibrium setting may allow life to evolve.



## Nanoparticles as structural and active elements for optoelectronics

**Andras Deak[1,2], Nguyen Quoc Khanh[2], Janos Volk[2], István Bársony[2], Enrico Da Como[1], Jochen Feldmann[1]**

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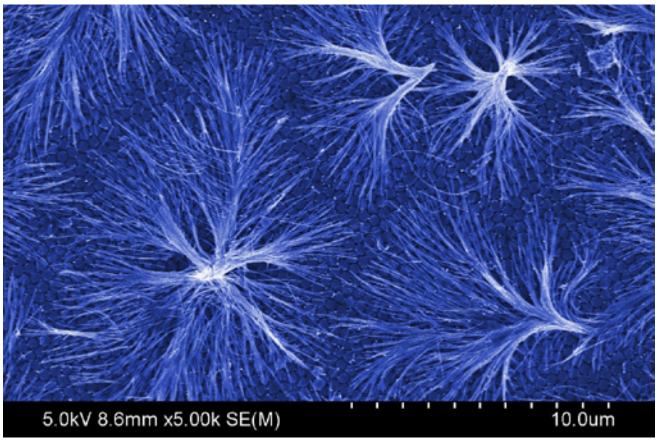
*[2]Research Institute for Technical Physics and Materials Science of the Hungarian Academy of Sciences, Budapest, Hungary*

Dielectric and metallodielectric core/shell nanoparticles were used to create inorganic and organic-inorganic thin film assemblies. These thin film structures might be interesting for optoelectronic applications, e.g. solar cells.

Extraordinary high aspect ratio (~400) ZnO nanowires were grown in one step on solid substrates by hydrothermal method (see Figure). Our novel concept is based on the nanoscale manipulation of the precursor concentration along the growing path of the nanowires by using a pre-deposited colloidal silica monolayer on top of the substrate. The nanoparticle layer serves as a nanoscale volume confining structure and as mass transport barrier at the initial stage of the nanowire growth. The prepared ZnO structure might find application, e.g. as large surface area electrodes in dye sensitised solar cells.



Extraordinary high aspect ratio (~ 400) ZnO nanowires grown with the aid of a monolayer of colloidal particles on solid substrate.

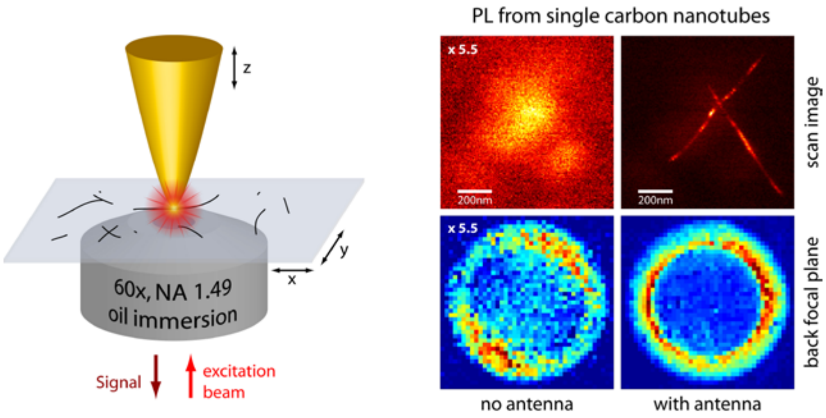
Organic-inorganic thin films were prepared from gold/silica core/shell nanorods and a blend of donor and acceptor type organics, generally used in organic bulk-heterojunction solar cells. We plan to investigate the interaction between the localized plasmonic near-field and the charge transfer state absorption present in these polymer blends. The possibility to change the aspect ratio of the gold core offers a facile way to tune the plasmon band position, while the thin silica shell isolates the metal from the organic matrix, preventing charge carrier recombination on the particle surface. Due to proper surface modification, the particles can be mixed directly with the polymer blend. This enables a more intimate interaction between the near field of the particles and the organic blend.

## TENOM – Optical Investigations with Enhanced Detection Sensitivity and Nanoscale Resolution

**Miriam Böhmler, Nicolai Hartmann, Carsten Georgi, Achim Hartschuh**

*Department Chemie & CeNS, LMU München, Germany*

Tip-enhanced near-field optical microscopy (TENOM) is a versatile method for the detection and investigation of nanoscale objects and nanostructured materials such as single molecules, carbon nanotubes, and semiconductor nanowires.[1,2] The highly enhanced electrical fields in the vicinity of a metallic nano-antenna lead to increased excitation and radiation rates in nearby quantum objects resulting in enhanced detection sensitivity and sub-diffraction spatial resolution of the optical signal. On our poster we illustrate two examples of our ongoing research using TENOM:



We present the first hyperspectral near-field images of a II-VI semiconductor nanowire showing Raman scattering as well as photoluminescence (PL) with a spatial resolution of about 25 nm. The photoluminescence energy was found to vary along the nanowire indicating nanoscale variations in the crystal structure. As second example, we present our investigations on the influence of the tip-antenna on the angular radiation pattern of individual single-walled carbon nanotubes' photoluminescence. The emitting nanotube can be described by a single in-plane point dipole. The near-field interaction between a nanotube and an optical antenna modifies the radiation pattern that is now dominated by the antenna characteristics.[3]

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*[2] K. F. Domke and B. Pettinger, "Studying Surface Chemistry beyond the Diffraction Limit: 10 Years of TERS", ChemPhysChem, 11, 1365 - 1373 (2010)*

*[3] M. Böhmler et al., "Enhancing and Redirecting Carbon Nanotube Photoluminescence by an Optical Antenna ", Optics Express, 18, 16443 (2010).*

## Fullerene Periodic Mesoporous Organosilica

**Kun Hou and Thomas Bein**

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Fullerenes, a set of hollow cage-shaped carbon molecules, have sparked remarkable interdisciplinary research activities in the past two decades, encompassing diverse fields of chemistry, physics, and materials science [1]. Since the availability of fullerenes in macroscopic quantities, a wide variety of chemically modified fullerene derivatives has been synthesized and outstanding magnetic [2] superconducting [3] electrochemical and photophysical properties have been reported [4,5]. These studies have triggered interest in fullerene applications such as solar cells, optical limiters, catalysts, superconductors, molecular electronics, etc. [6]

With this in mind, we conceived the idea of using functionalized fullerene as a building block for a new type of periodic mesoporous organosilica (PMO). PMO is a class of porous materials that posses both mesoporosity and tunable organic functional frameworks [7]. Because of the versatile properties and applications of fullerenes, the creation of a fullerene PMO offers the opportunity to impart these properties into a periodic porous framework that offers access to various guest molecules. For example, fullerene derivatives are among the most widely studied molecules in optoelectronics, therefore, creating a high surface area PMO with $C_{60}$ integrated into the pore wall may provide a new class of electroactive materials that could find applications in photovoltaics and electronics.

Here, we report the synthesis of electroactive fullerene PMO from a newly designed multifunctional fullerene precursor. The material was fully characterized by small angle X-ray diffraction (XRD), nitrogen sorption, transmission electron microscopy (TEM), and solid state NMR. Further, the electrochemistry of this new material was studied. Our results show that the framework composed of the multifunctionized fullerene derivative is still able to accept electrons at an appropriate bias voltage.

Acknowledgement: We acknowledge funding from the NIM Cluster (DFG) for this research.

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## Self Assembly of Titanium Oxide/Conjugated Polymer Mesostructures for Photovoltaic Applications

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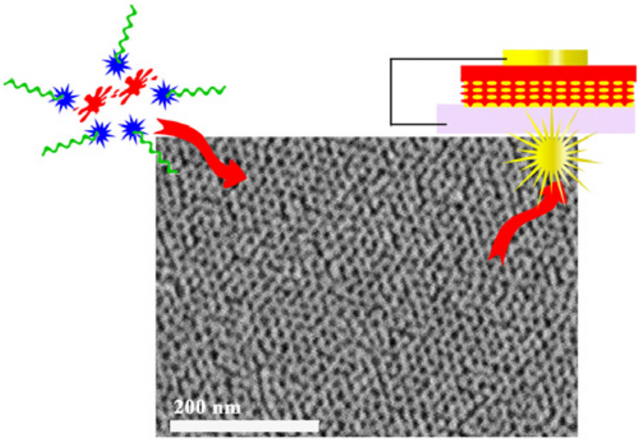
One of the greater challenges in the field of organic and hybrid organic/inorganic photovoltaics is to direct a donor-acceptor phase separation on a sub 20 nm length scale, and at the same time, obtain continuity and orientation of each individual phase on a much longer length scale. This hierarchical architecture is designed to enhance exciton dissociation into charge carriers, and provide a passway for efficient charge carrier transport to the electrodes.

To achieve this goal a titania precursor species, conjugated polymer (MEH-PPV) and an amphiphilic structure-directing agent (surfactant), are co-assembled in non-aqueous THF-based precursor solutions into 3D mesostructured continuous and interpenetrating organic/inorganic networks, with a ~10 nm phase separation between the conjugated polymer, the electron donor, and titanium oxide, the electron acceptor, as evident from SAXS and electron microscopy measurements,



Photocurrent generation through exciton dissociation at the organic/inorganic interface was studied by correlating device performance with photoluminescence decay and solid state NMR measurements. It was found that MEH-PPV chains present in the hydrophilic corona of the surfactant can efficiently transfer photo-excited electrons to the $TiO_2$ matrix leading to photocurrent, while MEH-PPV chains confined to the hydrophobic core are less probable to produce photocurrent. Therefore, judicious selection of the surfactant type and length provides a handle on the performance of the device through molecular control of the charge-generating organic/inorganic interface in MEHPPV/$TiO_2$ photovoltaic devices.

## Solid Solutions of the Organic Semiconductors Quinacridone/Quinacridonequinone: Electronic Properties and Phase Separation of Adsorbates

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Insoluble molecules such as organic pigments and semiconductors can be deposited on substrate surfaces under ambient conditions by applying the Organic Solid/Solid Wetting Deposition (OSWD) process [1]. When organic nanocrystals come into contact with a flat inorganic substrate surface, the process initiates the supramolecular self-assembly of monolayers. The behavior of the nanocrystal is comparable to liquid droplets wetting a surface. Using this OSWD process, molecules can be deposited either directly (dry) or with the aid of an organic binder.

We present how the semiconducting organic molecules of the solid solution Quinacridone/Quinacridonequinone (QAC/QACQ) assemble on graphite. No monolayer formation had been observed by using pure QACQ samples. However, using a solid solution of QAC/QACQ, a new pattern in addition to the known QAC pattern was formed. Our results indicate phase separation in the solid solution QAC/QACQ during the OSWD process and the assembly of different patterns, depending on the organic binder. For the investigation, Scanning Tunneling Microscopy (STM), Scanning Tunneling Spectroscopy (STS) and Density Functional Theory calculations (DFT) were used.

In conclusion, using solid solutions may broaden the applicability of the OSWD approach.

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## Spatially resolved optoelectronic measurements on organic thin film transistors

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Pentacene is a promising candidate for organic electronics and optoelectronic applications due to its high charge carrier mobility and strong absorption properties. Its optical properties are highly anisotropic. Therefore, the thin-film-phase texture of pentacene grains should be visible in polarized light due to anisotropic absorption behaviour. Absorption, being the initialising step to generate excitons, is a crucial point for the photoresponse of transistors. Consequently, the polycrystalline thin-film-phase texture might be directly related to the photoresponse of pentacene based OFETs.

Here we use local illumination of the transistor channel in a confocal laser scanning setup with submicron resolution providing excitation of single pentacene grains. The absorption of separate grains is found to be strongly dependent on the polarisation of the incident light, as expected. The observed luminescence image is very sharp and mirrors the thin-film texture. Therefore, absorption and luminescence match up perfectly. However, the spatially resolved photoresponse of the pentacene OFET shows an extrinsic structure which is blurred and almost independent of the polarization direction. To disentangle the underlying transport phenomena, time resolved photoresponse measurements were performed. Apart from a heat-induced homogeneous mechanism, these measurements also reveal two spatially inhomogeneous processes with different timescales. The obtained results for the photoresponse of pentacene based OFETs are explained by a model of triplet exciton assisted hole detrapping.

## Dynamics of Growing Cell Populations

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Many processes in tissues, such as cellular rearrangement, changes in cell shape and migration, can be described by mechanical cell models. Parameters like elasticity, contractility and cell-cell interactions have to be taken into account to describe structural organizations on a cellular level.

We use microstructured surfaces to analyse epithelia cell growth in a quantitative way and to develop biophysical models in alignment with experimental findings. To this end, we designed an experimental setup to prove the assumption of these models that a gradient in the homeostatic pressure is formed in a growing tissue. Cells were grown in channels and are limited to expand in more than two dimensions by the confinement of the walls. The resulting stress can be detected by the variation of area and height, depending on the position within the cell patch. In the second set of experiments, we study the dynamics of contour changes of a spreading and growing cell patch. Using removable PEG-DMA structures, we are able to prepare small cell patches of defined geometries. We investigate the evolution of the patch contour in the first hours of incipient cell migration. Image processing, in combination with stable transfected cell lines, permits the analysis of cell density, area distribution, and possible correlations with cell division events and, furthermore, the comparison with dynamic models of cell growth.

## Nanostructured solid-state solar cells

**Florian Auras, Norma K. Minar, Johann M. Szeifert, Angela Wochnik, Christina Scheu and Thomas Bein**

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Sunlight and its conversion into electric power represent a clean, abundant and renewable energy source, which is expected to cover a considerable part of the world's future energy demand. In order to achieve this goal, new types of efficient solar cells composed of abundant and non-toxic materials suitable for large scale production are required.

Solar cells based on mesoporous metal oxides have attracted much attention in the last few years. Here we report on solar cell designs based on mesoporous titania with very high surface area in combination with antimony sulfide as an inorganic light absorber. The interdigitated diode structure is completed by filling the remaining pore volume with a hole-conducting material such as poly(2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylenevinylene) (MEH-PPV).

Our research is focused on controlling the mesostructure and porosity of the titanium dioxide and on developing new methods for the deposition of the light absorbing materials. Tuning the thickness of the light absorbing layer and its morphology is essential in order to reduce recombination losses. For the production of such layers of only a few nanometers thickness, conventional chemical bath deposition and a non-aqueous variant of the subsequent ionic layer adsorption and reaction method are compared. A detailed investigation of the cells using electron microscopy and various spectroscopic methods reveals that the latter method gives much better control on the layer thickness and homogeneity. Fine-tuning of the absorber layer allows us to enhance the electron diffusion length and thereby achieve higher photovoltaic efficiencies.

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## High-resolution Raman spectroscopic study of defects in double- and single-walled carbon nanotubes

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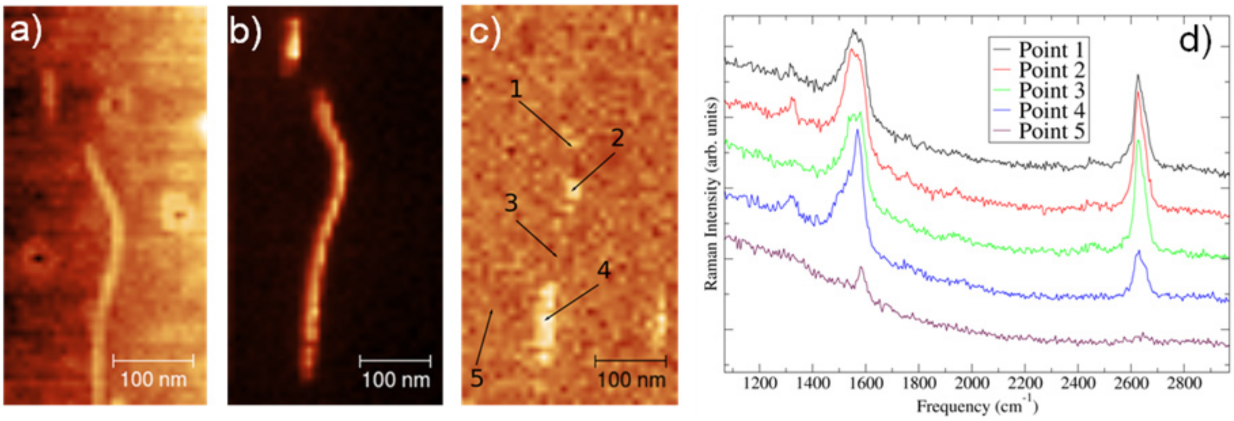
The introduction of localized defects in carbon nanotubes is a way to change the intrinsic properties of these nanostructures and perhaps to create new nanodevices. Tip-enhanced Raman spectroscopy (TERS) provides sub-diffraction spatial resolution (<20 nm) by locally increasing signal intensities and this technique is ideally suited for spectroscopic imaging of nanoscale features. In this work we study defects in double-walled carbon nanotubes (DWNT) as well as in metallic single-walled carbon nanotubes (SWNTs) using TERS focusing on two fundamental questions: First, what is the Raman signature of different types of defects and second, what is the decay length of these signatures?

The defects in the DWNTs were induced by 100 keV C+ ion-bombardment with increasing ion-fluences. Ensemble spectra show increased defect-induced D-band scattering as well as a substantial broadening of the G-band. Using TERS on the same samples we identified fully pristine and fully defective nanotubes in agreement with the ensemble measurements. For DWNT exposed to small ion-fluences we found some spatially localized defects (Fig. 1(c)): the decay length of the D-band scattering at point 1 is substantially smaller than 20 nm, the spatial resolution of our experiment. We also noted a correlated shift and a splitting of the G-band (Fig. 1d), a feature that is still under investigation. Finally, local defects in metallic SWNTs were photo-induced intentionally by the strong tip-enhanced optical fields. The created D-band scattering signal thus produced was found to be highly localized within our spatial resolution as well.

Fig. 1. (a) Topography, (b) G-band and (c) D-band spectroscopic images and the (d) respective Raman spectra.



## Synthesis and functionality of ordered hierarchical meso-macroporous titania systems

**Benjamin Mandlmeier**, **Thomas Bein**

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Hierarchical mesoporous-macroporous materials are of interest when transport and interfacial processes need to be balanced and optimized. Here we report on the design and functionality of hierarchical titania materials intended as anodes in dye-sensitized solar cells (DSC). The macroporous structural features are generated by hard templating with polymer spheres (d > 50 nm), while the mesoporous structures are obtained via soft templating with lyotropic liquid crystalline surfactant phases interacting with sol-gel derived titania networks. The mesoporous crystalline titania acts as an efficient light harvesting and charge separation component due to its high interface area enabling significant uptake of sensitizer dye, while the macroporous titania phase provides an efficient transport of the collected charge due to its high crystallinity and high electron mobility. Specifically, the strategy for generating such hierarchical structures involves preparation of inverse opal titania layers by the hard templating technique and then filling the interstitial macroporous voids with various precursors for the mesostructured titania phase using an evaporation-induced self-assembly (EISA) approach. Figure 1 illustrates the general synthesis procedure of periodic hierarchical macroporous-mesoporous nanostructures (HMM).

HMM titania nanostructures were characterized in detail regarding crystallinity, porosity and morphology obtained after each step of the fabrication procedure. The HMM titania systems were also investigated as anodes in DSCs and show a strongly increased efficiency compared to the open macroporous titania anodes.

Acknowledgement: The authors acknowledge funding for this project in the context of the Excellence Initiative (DFG).

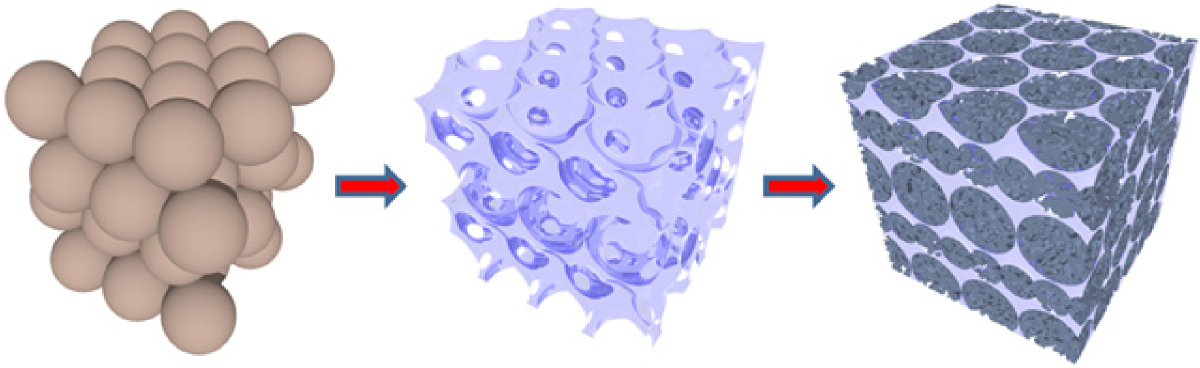

Figure 1: Scheme and of the three-step bottom-up approach towards HMM. (left) Sphere assembly into colloidal crystals. (middle) Material intrusion into the interstitial voids and network formation after template removal. (right) Post-modification of the inverse opal with mesoporous titania.

## Photocatalytic hydrogen production by visible-light illuminated dye-sensitized $TiO_2$ nanoparticles in solution

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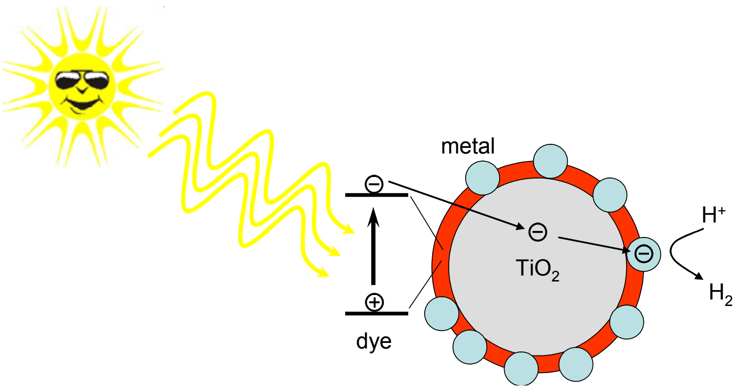
P25 $TiO_2$ nanoparticles have been functionalized by wet-impregnation with metal catalyst nanoparticles (palladium and copper) and subsequently sensitized with perylene dyes (ID28 and derivatives). The nanoparticles were then transferred to aqueous environment and the dispersion was illuminated by visible light from 18W Biolux lamps. Cutoff filter at 420nm was used to eliminate UV light. The gas chromatography analysis of the gas phase (headspace) shows significant hydrogen generation from photocatalytic reduction of $H^+$ ions on the metal catalyst centres. In this work we present the results of studies of effect a number of parameters such as: pH, nanoparticle concentration and choice of sacrificial donor (i.e. hole acceptor) and role of additives to the dispersion ($Li^+$ ions) on the overall efficiency of the process.



## Radio Frequency Characterization of Gate-Defined Triple Quantum Dots

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Quantum dots (QDs) have been proposed as the fundamental units for quantum information processing, the qubits [1]. Gate defined QDs can be fabricated by means of industrial methods and have the advantage of a straightforward scalability to many coupled QDs and a full tuneability. They allow initialization, manipulation and read-out of the single qubits as well as a controlled coupling between qubits [2].

Our nano-devices are defined by means of Schottky gates on the surface of a GaAs/AlGaAs heterostructure containing a two-dimensional electron system. The measurements are performed in a dilution refrigerator near its base temperature of 15 mK. Here we present a novel design of a fully tuneable electrostatically defined serial triple quantum dot in which the charge configuration as well as all tunnel barriers can be manipulated via control gates (compare Figure a).

Coherent transport by adiabatic passage (CTAP) has been proposed as a robust and fast protocol to couple distant qubits [3]. For CTAP a detailed knowledge and precise control of the interdot tunnel couplings at radio frequencies is essential. In our experiments we characterize the triple-quantum dot structure in the fewest electron regime using a weakly biased QPC as detector. We employ an ultra fast (sub-nanosecond) rf pulsing scheme to estimate an upper bound of the tunneling frequencies between the quantum dots, while we measure their average electron occupancy [4]. In addition, we demonstrate the advantages of our novel gate design, namely a better tuneability which allows for instance to easily remove significant asymmetries.

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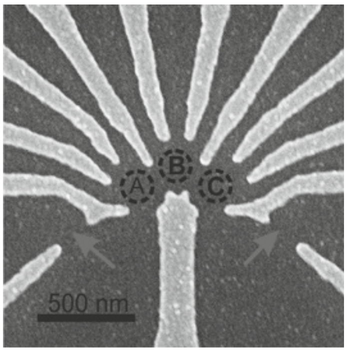
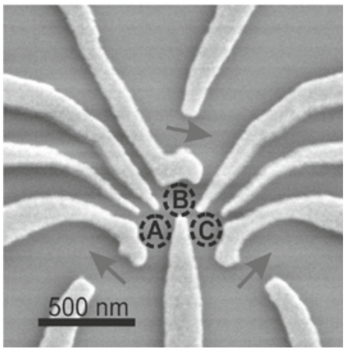


Picture a) Scanning electron micrograph of a device nominally identical to the investigated one. Circles depict the estimated position of the quantum dots A, B and C. Arrows the direction of the current through the quantum point contacts.



Picture b) Scanning electron micrograph of a device with the former gate architecture. Circles depict the estimated position of the quantum dots A, B and C. Arrows the direction of the current through the quantum point contacts.

## Gold nanoparticles inserted into NiOOH as a strategy to enhance sensitivity and stability

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Nickel hydroxide electrodes have great potential as sensors for organic analytes and they have been applied for determination of acetylsalicylic acid, urea, glicin and others. However, the nickel hydroxide structure is changed during oxi-reduction cycles, losing progressively its activity. The modification of this material with metallic nanoparticles could not only enhance the stability of the structure but also raise the sensitivity of the electrode. Looking for the development of a sensor with high performance, this work shows the insertion of gold nanoparticles in nickel hydroxide films. All the films were electrodepositated with time varying from 10 to 120 s onto bare glassy carbon electrode from a $Ni(NO_3)_2$ solution. In those films with gold nanoparticles, was added to the nickel nitrate solution, 50 microL of gold colloidal suspension. Three different diameters of the nanoparticles were tested, 5, 10 and 20 nm. Then, the film was submitted to 30 voltammetric cycles to evaluate the magnitude of the oxidation current and the stability of the material. The Figure 1 presents the cyclic voltammograms of two modified electrodes, one with only NiOOH and the other one with AuNP/NiOOH. The modified electrode AuNP/NiOOH presents a higher current than the pure film. This effect can be attributed to the increment in the electron transfer in the electrode. Once the current is raised, the sensitivity of the AuNP/NiOOH electrode is better compared to the pure film.

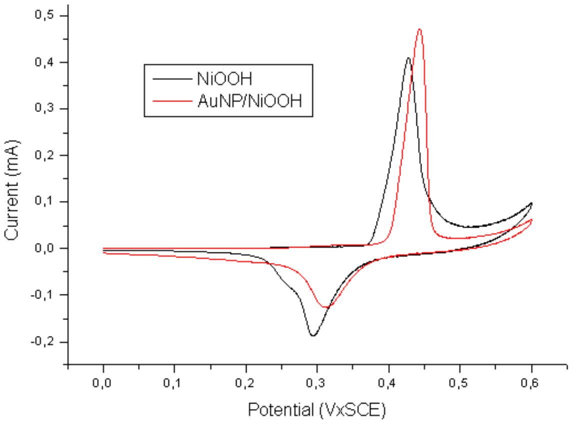

Fig. 1: Cyclic voltammograms of the nickel hydroxide films: pure (black line) and containing gold nanoparticles (red line).

## A new functional triazine framework based on N-hetrocyclic building blocks

**Stephan Hug, Michael Tauchert, Shen Li, Bettina Lotsch**

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Covalent organic frameworks (COFs) – as opposed to metal organic frameworks (MOFs) – have the advantage of lightweight building blocks, strong covalent bonds, high chemical and thermal stability, and high surface areas [1-2]. Recently, triazine-based COFs (dubbed CTFs, covalent triazine frameworks) have been used for heterogeneous catalysis by loading with platinum salts and palladium nanoparticles [3-4]. The presence of triazine moieties proved to be beneficial for the selective bonding of the catalytic agents. In order to provide more specific and strong binding sites for a large variety of metal ions, we have designed a COF based on 5,5'-dicyanobipyridine linkers, where the bipyridine unit acts as a scaffold to site-selectively coordinate the metal cations. This type of binding ensures a "homogeneous" environment of the metal ions in the framework, which on the other hand is highly robust and insoluble in essentially all organic solvents and even in strong acids. A typical synthesis was carried out under ionothermal conditions at 400°C using $ZnCl_2$ as a lewis acidic trimerization catalyst [5]. The surface area of the resulting microporous frameworks is in the range of 1000 $m^2$ $g^{-1}$, and the products are chemically inert and thermally stable. Loading experiments with platinum and palladium salts gave adsorptions of those salts up to 50 wt%. Investigations into the catalytic activity of the metal-doped frameworks in methane oxidation and hydrogenation reactions are underway.

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## A versatile, drift-stable SPM with stick-slip coarse approach for molecular self-assembly studies

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Here we present a low-drift Scanning Tunneling Microscope (STM) with a stick-slip based coarse approach for ambient use. The microscope is ideally suited to study supramolecular self-assembly on surfaces with submolecular resolution.

By virtue of design and choice of materials, lateral drift is minimized, thereby allowing for precise measurement of lattice parameters and intermolecular distances. Integration of a modified attocube linear positioner allows for a fully automated and crash free coarse approach in typically less than two minutes. The STM presented combines the high stability of the beetle (Besocke) design with ease of use.

Besides that the instrument features a fully accessible tunneling junction. This can be used for in-situ deposition of molecules from solution by means of a micropipette while the sample surface is continuously imaged. By means of this novel in-situ deposition technique, new types of experiments become feasible. For instance dynamic behavior in supramolecular host-guest chemistry can be studied. Also the instrument can by used as Atomic Force Microscopy with a quartz tuning fork.

## The Role of Water in Protein Binding to Functionalized Inorganic Surfaces

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[7]*Advanced Diamond Technologies, Inc.*

Antibody-based sensors offer the potential for highly-selective and highly-sensitive pathogen detection. Recent experiments [1] have demonstrated superior performance of immunosurfaces based on functionalized ultrananocrystalline diamond (UNCD) in comparison to conventional functionalized-silica substrates. Nevertheless, both types of immunosurfaces have shown a steady decline of the antibody activity over time. We hypothesized that such loss of activity is caused by nonspecific binding of antibodies to immunosurfaces. To investigate how the choice of the substrate and its functionalization affects the properties of the immunosurfaces, we carried out molecular dynamics simulations of functionalized UNCD and silica in aqueous salt solution. The simulations have demonstrated that the structure of water near the immunosurfaces highly depends on the substrate material and the density and length of the functional groups. To quantitatively determine the effect of water structure on the proteins affinity to the immunosurfaces, we have characterized the effective interaction potential between amino acids and the UNCD and silica substrates, with and without the functionalization layer. Our results demonstrate a considerable increase in binding affinity of amino acids due to the loss of functional groups or a change in the surface chemistry of the substrate."

## TEM investigations on thin $Fe_xO_y$ films on $Al_2O_3$

**Teresa Dennenwaldt[1], Markus Döblinger[1], Maike Lübbe[2], Wolfgang Moritz[2], Rossitza Pentcheva[2], Tzipi Cohen[3] and Christina Scheu[1]**

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The investigation of thin magnetic films and their interfaces is the current topic of scientific interest. The magnetic properties can be tuned by controlling their domain structures (i.e. orientation relationship), grain boundaries and their interfaces. The chemical compositions/variations locally at these interfaces/domain walls play a crucial role in determining the functional properties of the thin films. To understand the correlation between properties, synthesis and structure, characterization methods with a high spatial resolution are required on the structural-chemical composition and the binding properties. We used Transmission Electron Microscopy (TEM) for analysis at nanoscale.

In this work, Molecular Beam Epitaxy (MBE) grown thin films of hematite ($\alpha$-$Fe_2O_3$) and ilmenite ($FeTiO_3$) on sapphire substrate ($\alpha$-$Al_2O_3$) were investigated using different TEM techniques. With the help of Conventional TEM (C-TEM) methods, the local microstructure, the morphology, the defects and the thickness of the thin films were investigated in detail. Diffraction pattern provide information on crystal structure of the thin films and their orientation relationship with substrates. With High Resolution TEM (HR-TEM) and High Angle Annular Dark Field-Scanning TEM (HAADF-STEM) the atomic structure, the defects and the interfaces were characterized. In order to get the information on chemical composition and binding properties, methods like Energy Dispersive X-ray Spectrometry (EDS) and Energy Electron Loss Spectroscopy (EELS) were used.

Our results show that the thickness of the thin films was much higher than expected and that the surface was extremely rough which indicates an island growth process. The thin films are polycrystalline. From the diffraction pattern we confirm the presence of two different phases (hematite and magnetite). While surface X-Ray Diffraction (XRD) showed reflections due to an epitaxial growth of hematite and magnetite islands, the TEM images showed a large number of domains without any orientation relation. The valence state of Fe and Ti was studied within the grains by inspecting the Fe- and Ti-$L_{2,3}$-edges with EELS. In the next step these investigations will be performed at interfaces and domain walls. The results are very useful to apprehend the magnetic properties of thin films at the nanoscale.

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## Detection system for lateral flow immunoassays

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In the developing world, there is a lack of convenient and accurate point-of-care tools that can detect and diagnose diseases in remote or impoverished settings. Lateral flow immunoassays (LFIA) have been used as an appropriate technology to a wide variety of point-of-care or field applications. However, the challenge of these test systems is the detection limit, which should be reliable and precise at the same time. Furthermore, the system has to be inexpensive and should be based on visual detection. Coupling of coloured nanoparticles to the detection molecule is the most useful technique for an immediate read-out of the test. This work compares and identifies different coloured nanoparticles that provide the highest visual signal. As a proof of concept, they will be used as a LFIA detection system for Dengue fever (DF), a viral disease transmitted by Aedes mosquitoes. In pre-experiments, conjugates of streptavidin with colloidal gold, silver coated gold nanoparticles, blue latex beads and carbon black were tested with different concentrations of biotinylated albumin solutions previously immobilized onto nitrocellulose membranes. Grayscale values from scanned membranes for all tested nanoparticles are shown in figure 1. Carbon black particles provide the best signal to noise ratio and a considerable signal variation by changing the biotinylated albumin concentration. The intensity difference between carbon black and silver coated gold nanoparticles, the second label in signal intensity, is even higher than 50%. Based on these results, carbon black was chosen as detection label for non-structural glycoprotein 1 (NS1) of the Dengue virus. Anti-NS1 monoclonal antibodies were immobilized on carbon black via covalent mechanism and tested in DF infected blood. A comparison with commercial diagnostic tests for DF, based on gold nanoparticles, showed that carbon black particle set up improves the detection limit for LFIA tests.

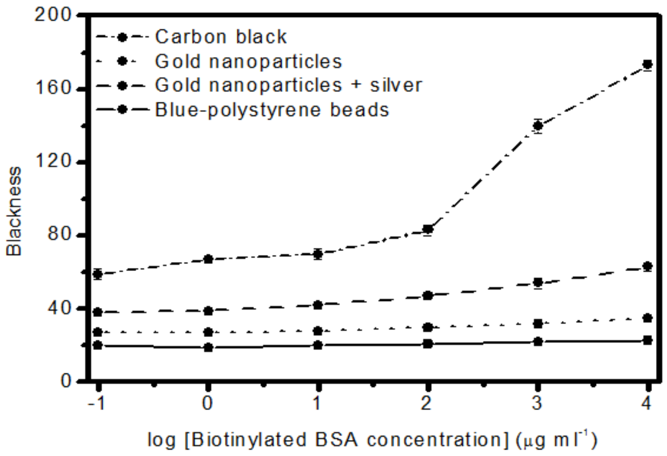

Fig. 1: Curves comparing the blackness intensity for different labels according biotinylated albumin concentration. Expanded area within the graph shows blackness variation for all labels exluding carbon black.

## Single-Molecule Force-Clamp Spectroscopy Reveals the Structural Topology of Titin Kinase

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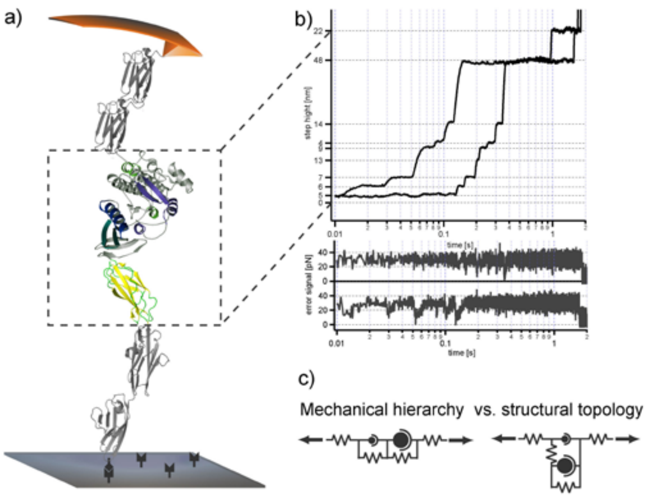
[2]*Center for Integrated Protein Science Munich*

The architecture of proteins that underlie mechanical stress in their natural environment and have to fulfil a special task under these conditions is of special interest since it shows how evolution has adapted for this need. As it was recently demonstrated in our group with AFM measurements, the muscle enzyme titin kinase can be mechanically activated [1]. In contrast to many other molecules that have been studied with single-molecule force spectroscopy it does not unfold in one step only but exhibits up to six energy barriers that have to be overcome until the protein is completely stretched. After the first two energy barriers the sterically shielded binding side is opened and accessible for ATP [2].

Here we demonstrate that structural topology rather than mechanical hierarchy stabilizes the elements of titin kinase. Single-molecule force-clamp experiments show, that the structural elements are shielding one another and stress is only applied to one element at a time. Such the enzyme can make use of mechanical induced topology changes for signal transmission without loosing its structural integrity.



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## Hybridisation kinetics is different inside cells

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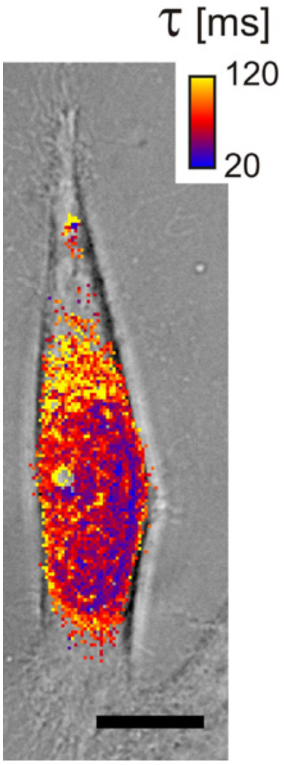
It is generally expected that the kinetics of reactions inside living cells differs from the situation in bulk solutions.

Macromolecular crowding as well as specific binding interactions could change kinetic behaviour of reactions. Here we show spatially resolved measurements of DNA hybridization kinetics in single living cells with a range of 10 µs to 1 s by a combination of laser-driven temperature oscillations and stroboscopic fluorescence imaging.

A quantitative analysis of the concentration dependence revealed several-fold accelerated kinetics as compared to free solution for a 16 bp probe and decelerated kinetics for a 12 bp probe. We did not find significant effects of crowding agents on the hybridization kinetics in vitro. The presented imaging modality of TOOL (Temperature Oscillation Optical Lock-in) microscopy allows to probe biomolecular interactions in different cell compartments in living cells for systems biology.



## Optoelectronic properties of two-dimensional gold nanoparticle arrays

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The field of plasmonics deals with the interaction of light with metal clusters. It has drawn a lot of interest in recent years due to possible applications for surface enhanced Raman spectroscopy and biosensing. The absorption of light by nanoparticles induces surface plasma oscillations of the conduction electrons. At first, this leads to a strongly enhanced electrical field at the surface of the particles and, secondary, the plasmons decay and heat up the particles. We use self-assembled two dimensional arrays of alkane coated gold nanoparticles to investigate the impact of these two effects on the transport properties of such arrays.

By probing the photoconductance of a contacted gold nanoparticle array we find a clear enhancement of the photoconductance at the surface plasmon resonance. This can be explained by bolometrically enhanced tunnel rates between adjacent nanoparticles. [1] Furthermore, finite difference time domain simulations have shown a strong field enhancement between the nanoparticles in the array under optical excitation of the surface plasmons. This field enhancement leads to a strongly increased optoelectronic response of the nanoparticle array. [2]

We acknowledge a fruitful collaboration with M. Calame and C. Schönenberger. This work has been supported by the "Deutsche Forschungsgemeinschaft" through project HO 3324/2, the excellence program "Nano Initiative Munich" (NIM), and the Center for NanoScience (CeNS) in Munich.

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## TEM investigation of nanostructured hybrid solar cells

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Increasing the photo-reactant interface of hybrid solar cells is a major aim to improve their efficiency, consequently diverse methods of nanostructuration of polymer-metaloxide interfaces are pursued and under investigation. One possibility is a highly-ordered growth of inorganic nanowires or nanotubes which form arrays on differing substrates. Due to their dimension in nano scale, a complete elucidation of their structure is not possible using conventional techniques like X-ray Diffractometry (XRD) or Scanning Electron Microscopy (SEM).

Thus, in this study Transmission Electron Microscopy (TEM) is used to investigate micro- and nanostructure of $TiO_2$ nanowires and nanotube arrays which act as n-type semiconductor. They are grown on conducting transparent substrates by diverse fabrication methods like hydrothermal growth, via anodized alumina templates or anodizing of Ti layers. To provide complete solar cells, these nanostructures are filled by polymers like P3HT which serve as p-type semiconductors and e.g. Ag is deposited on top as counter electrode.

In the present study, Bright-Field (BF) TEM is used to explore the alignment of arrays and layers, Electron Diffraction (ED) for the investigation of local and macroscopic crystallinity and High Resolution TEM (HRTEM) provides understanding of interfaces and a correlation to their properties. Additionally, analytical TEM is used for further investigation, whereupon Energy Dispersive X-ray Spectroscopy (EDX) is used to detect impurities while Electron Energy Loss Spectroscopy (EELS) gives an understanding of chemical properties like chemical bonding of elements and therefore their chemical composition. All of these techniques are possible with high spatial resolution so that the location of defects and inconsistencies can be determined precisely.

First results show crystallinity of the nanowires as predicted, but also demonstrate a need for improvement of purity and arrangement of the arrays.

Note: Fabrication and physical properties of the $TiO_2$ nanotube-based solar cells are described in the contribution "Device Physics of Nanostructured Hybrid Solar Cells" by J. Weickert et al.

## Spatiotemporal formation of the Konde screening cloud

**Alexander Hoffmann, Stefan Kehrein**
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The Kondo model is a long known model to simulate magnetic impurities in a metal. Its equilibrium spin-spin susceptibilities are well known. We study this quantities in the non-equilibrium case.

We calculate the time dependent spin-spin-susceptibility between the impurity and the conduction band spin an a sudden switching on of the interaction to study the formation of the Kondo screening cloud. To this end we bosonise the Kondo model and then refemionise at the Toulouse point mapping it on the resonant level model.

## Applications of the Molecular Force Assay on Living Cells

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Surface receptors and their interactions are in focus of biomedical research as they play a fundamental role in signal transduction and are involved in cancer development and progression. The molecular force balance on living cells offers the perspective to access the binding properties of such receptors in their physiological environment. The method relies on the well-established principle of the molecular force assay (MFA) that was so far only applied on molecules immobilized on surfaces. It is an ensemble measurement that analyzes binding forces of receptor ligand interactions on a single molecule level by directly comparing the binding force of interest to a known reference interaction. Reference and probe are clamped in series between two surfaces. When separating the surfaces, the molecular complex with the weaker bond is more likely to rupture. A fluorescent label at the reference complex indicates the outcome of the experiment. This highly parallel method ensures to measure specific binding of a cell surface receptor to its ligand by exertion of a certain reference force that exceeds the strength of unspecific interactions. Thus, the introduced assay is a promising method that is not only capable of screening for various receptors on the membrane of a certain cell line in one experiment but can also estimate the binding forces of those interactions.

## Assembly of thin mesoporous titania films for hybrid solar cells

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Organic photovoltaic materials are under intensive study for potential applications in low-cost, large-area solar cells. Although all-organic systems such as polymer/fullerene blends are receiving high interest, these systems suffer from poor photostability of the two organic compounds and low mechanic stability of the active layers through phase segregation.

One promising alternative approach is to use a nanostructured *inorganic* semiconductor as the electron-transport component. Crystalline titanium dioxide is an attractive material in this context on account of the low cost, good stability, ease of fabrication and the potential for controlling the film morphology on the nanoscale.

Recently, we have developed a "brick and mortar" preparation strategy combining the advantages of particulate approaches and templated sol-gel processes by fusing preformed titania nanocrystals with surfactant-templated sol-gel titania, which acts as a structure-directing matrix and as a chemical glue.[1] Thin films prepared in this way require a significantly lower temperature for crystallization and retain their mesoporous structure.

As electron donor phase poly[2-methoxy-5-(2'-ethyl-hexyloxy)-1,4-phenylene vinylene] (MEH-PPV) was chosen based on its long exciton diffusion length (20 nm), high hole mobility and good absorbance in the visible range of the light spectrum (400-600 nm). The assembly of the organic and inorganic phase to build efficient photovoltaic devices should yield a high interface area between titania and MEH-PPV to provide a large number of exciton dissociation sites. Our approach to achieve high pore filling of the titania electrode and improved photovoltaic characteristics is to prepare the conjugated polymer in situ, via the thermally-induced Gilch route. We will discuss the structural characteristics and the solar cell performance of these inorganic/organic hybrid solar cells.

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Acknowledgement: The authors acknowledge funding for this project in the context of the Excellence Initiative (DFG).

## Synthesis of crystalline mesoporous titania films through surfactant-assisted assembly of ultrasmall anatase nanocrystals for applications in dye-sensitized solar cells

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Ultrasmall, crystalline and highly dispersible anatase nanoparticles were prepared in a microwave-assisted non-aqueous sol-gel procedure with a specially designed temperature profile. These nanoparticles were employed as building blocks for the preparation of mesoporous thin films by an evaporation-induced self-assembly (EISA) approach. The mesoporous films were characterized by TEM, SEM and SAXS to determine the morphology of their mesostructure. The mesoporous nanoparticle films exhibit an open porous system with high surface area, pore volume and good molecular accessibility in sorption measurements. Additionally, the crystalline nature of the films and their potential for energy storage is shown by lithium insertion. Using this method and supported by X-ray diffraction, a seeding effect of the incorporated nanoparticles in the mesoporous walls compared to samples from templated sol-gel approaches could be demonstrated. The high crystallinity, high surface area and good accessibility of the pore system make these films promising candidates for applications as photoanodes in dye-sensitized solar cells (DSC). Films of around 8 μm in thickness were produced by a multiple layering technique and showed high conversion efficiencies up to 7.7 % with a volatile electrolyte system. Future experiments with thinner films and ionic liquids as electrolytes will show possible advantages of these mesostructured anodes compared to the common particulate-based titania electrodes.

Acknowledgement: The authors acknowledge funding for this project in the context of the Excellence Initiative (DFG).

## Electronic contacts to GaAs nanowires by FIB-deposited metals

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Focused ion beam (FIB) lithography is a field of growing interest, as it allows etching as well as the deposition of insulating and conducting films on a submicron scale. We show that nanostructures, such as GaAs nanowires [1,2], can be electronically contacted using ion beam induced deposition (IBID). For our work, we used a 30kV $Ga^+$ FIB system (NVision40, Zeiss) together with tungsten hexacarbonyl [$W(CO)_6$], a common precursor for conductive deposits. Generally, the yield of the presented method strongly depends on several beam and scanning parameters, such as beam current, pixel size and dwell time, as well as substrate composition. For the purpose of electric contacts to semiconductor nanowires, a low resistivity and a low contact resistance to the gold electrodes is required. We have found resistivity of tungsten deposits to be ≈ 5 Ωμm, and the contact resistance to vary between 30 Ω and 100 Ω.

We thank A. Fontcuberta i Morral, G. Abstreiter, D. Spirkoska, C. Ruppert, and M. Betz for a fruitful collaboration regarding optoelectronic characterization of semiconductor nanowires. We gratefully acknowledge financial support by the Center for Nanoscience (CeNS), the Deutsche Forschungsgemeinschaft DFG through the excellence program "Nanosystems Initiative Munich (NIM)", the DFG grant HO-3324/4, and the SPP 1391.

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*[2] C. Ruppert, S. Thunich, G. Abstreiter, A. Fontcuberta i Morral, A.W. Holleitner, M. Betz, Nano Letters 10, 1799-1804 (2010).*

## Single molecule pull-down

**Ankur Jain[1], Ruijie Liu[2], Biswarathan Ramani[2], Edwin Arauz[3], Yuji Ishitsuka[4, 5], Kaushik Ragunathan[1], Jie Chen[3], Yang Xiang[2, *] and Taekjip Ha[1, 4, 5, *]**

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Protein-protein interactions form the cornerstone for most biological pathways. Governed by numerous factors, same protein can associate with a host of different proteins and exhibit diverse functionality in a specific physiological setting. This heterogeneity in protein interactions is difficult to probe using bulk assays like Western blots. We present a single molecule assay for direct visualization of in vivo biomolecular complexes. Protein complexes are immunoprecipitated directly from cell and tissue extracts. The proposed interacting partners are labeled with distinct fluorophores. Using multicolor fluorescence colocalization with single fluorophore sensitivity, we are able to determine the complex composition under physiological stimulations. Discrete photobleaching events provide information on the complex stoichiometry. The method is amenable for pull down of endogenous proteins. Pulled down complexes can be used for single molecule functional analysis. Single molecule immunoprecipitation provides a rapid, sensitive and robust platform for analyzing multimeric protein assemblies in different biological pathways.

## Bayesian inference based evaluation of DNA hairpin dynamics

**Wolfgang Kügel, Adam Muschielok and Jens Michaelis**

*Lehrstuhl für Physikalische Chemie I, Department Chemie, Ludwig-Maximilians-Universität München*

Fluorescence-correlation-spectroscopy (FCS) combined with FRET is a powerful tool to analyze dynamics in biological systems. In comparison to other approaches this technique is not limited to a narrow rate-window but dynamics from the ns to s time-scale can be investigated. However, the key problem is to extract the rates hidden in the correlation curve by fitting a set of parameters. A number of different fitting approaches have been described in recent years but the extraction of relevant information is still limited by the fact that the set of starting values chosen predefines the result. This happens as different sets of parameters result in a number of fitting curves describing the data equally well. To evaluate and weigh all possible fit results for our set of data we have used a Bayesian Inference approach and globally evaluated all information available. A first application of this approach will be presented based on a representative selection of different FRET pairs bound to a hairpin DNA showing how dye selection can influence the rates of hairpin opening and closing.

## Near-field spectra from broadband-infrared nanoscope

**Sergiu Amarie,* and F. Keilmann,**

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Basic material contrasts from either molecular "fingerprint" vibrations and crystal phonons, or from conductivity features make a full mid-infrared spectroscopic operation of scanning near-field optical microscope (SNOM) highly desirable. We have now achieved this goal by employing a compact dual-output Er-fiber system and difference-frequency generation. Thus we demonstrate 300 $cm^{-1}$ wide spectra in the 700-1400 $cm^{-1}$ mid-infrared region taken from single pixels of about 20 nm size. Strongest responses come from crystals in the phonon region. We show the resulting phonon-resonances of numerous crystals such as $CaCO_3$, SiC, $Ca_5(PO_4)_3(OH)$, $SiO_2$, and $\alpha$-$SiO_2$. Quantitative amplitude and phase spectra are compared with theory. The near-field phonon resonance is a robust and well-understood feature whose bright and sharp signatures can specifically highlight and identify polar materials in the nanoscale imaging of heterogeneous composites. Our immediate goal is to study hard biological matter such as bone and teeth.

## Excitation Transfer of Light Harvesting Complex 2 using Dissipative Quantum Dynamics

**Johan Strumpfer** and **Klaus Schulten**

*Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, ILCenter for Biophysics and Computational Biology, University of Illinois at Urbana-Champaign, Urbana, IL*

The dynamics of excitation energy transfer within the B850 ring of light harvesting complex 2 from Rhodobacter sphaeroides and between neighboring B850 rings is investigated by means of the hierarchy equations of motion for dissipative quantum mechanics. The assumption of Boltzmann populated donor states for the calculation of inter-complex excitation transfer rates by generalized Förster theory is shown to give accurate results as intra-complex exciton relaxation occurs in about 1 ps. Utilizing generalized Forster theory, the primary channels of exciton transfer between B850 rings are found to be the five lowest-lying exciton states with the non-850 nm states making significant contributions to the total transfer rate.

## Carrier relaxation in a single flake of bi-layer graphene studied by ultrafast spectroscopy

**Enrico Da Como, Thomas Limmer, Arjan Houtepen, Jochen Feldmann**

*Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität, Munich, Germany.*

In this communication, we report the first experiments probing the carrier relaxation on a single flake of bi-layer graphene with femtosecond resolution. Bi-layer graphene flakes have been obtained by mechanical exfoliation of natural graphite and do not show signatures of extrinsic carrier doping. We have probed carrier relaxation by ultrafast pump-probe spectroscopy in the femtosecond time scale, with a unique range of probe energies spanning between 1.2 to 0.25 eV. This allows us for obtaining snapshots of the carrier population distribution after the initial photoexcitation pulse at 1.55 eV. By modeling the carrier distributions as two separated Fermi-Dirac distributions for electrons and holes we extract carrier temperatures and cooling rates. Our analysis shows that carriers loose half of their energy within the first 500 femtoseconds by carrier-phonon scattering. The results are relevant for graphene optoelectronic devices and give valuable information for the understanding and modeling of hot carrier transport in ultrafast graphene devices.

## TEM characterization of nano-morphologies in solid state solar cells

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The development of new semiconductor materials for solar cells is a highly active area of research, aimed to simplify the manufacturing processes and to reduce production cost. In our work we develop nanocrystalline thin-film solar cells based on mesoporous materials, with different absorber materials and solid hole conductors. The working principle of these solar cells is as follows. The incident light is absorbed by a thin semiconductor layer and produces electron-hole pairs. The electrons are then transported through the oxide to the anode and the holes via the hole conductor to the cathode. The resulting voltage can be used to operate an external device.

As an electron conductor, mesoporous $TiO_2$ is used. The mesoporous oxide has a large surface to volume ratio, which can lead to efficient charge-carrier separation. In the present work, different mesoporous 3D-structures of $TiO_2$ were investigated, produced by different synthesis methods. These different mesoporous films were analyzed with respect to their structure, phase, crystallinity and grain size using various transmission electron microscopy (TEM) and spectroscopy based techniques. The composition and purity of the materials were analyzed with energy dispersive X-ray spectroscopy (EDS) and electron energy loss spectroscopy (EELS). To complete a working solar cell, the mesoporous $TiO_2$ is coated with absorber materials and filled with a solid hole conductor. Again TEM-based techniques are valuable tools to get detailed insights into the impact of nanostructure and morphology on the efficiency of the working solar cells.

Acknowledgement: The authors acknowledge funding from the NIM-cluster and from LMUexcellent for this work.

## Single-Molecule Spectroscopy on DNA Origami

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Recent developments in DNA nanotechnology facilitate a new degree of control to place arbitrary objects. By employing a technique termed DNA origami, 2- and 3-dimensional structures on a nanometer to micrometer scale can be designed and built by self assembly of individual DNA strands. In addition, some of these strands can be modified to attach objects of interest such as fluorophores or nanoparticles to the construct at specific sites. A unique capability of the DNA origami technique is that it allows the placement of these objects with a high precision that is at best on the range of single nucleotides, i.e. in the sub-nanometer range. Based on the vision of complex self-assembled nanosystems, we have immobilized fluorophores on DNA origami structures and resolved them by superresolution microscopy and single-molecule FRET. Additionally, employing these DNA nanostructures as a “molecular breadboard” offers the opportunity to study the effect of nanoparticles on the fluorescence properties of fluorophores such as enhancement of fluorescence intensity.

## Optically active periodic mesoporous organosilica in confined environments

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Periodic mesoporous organosilica (PMO) has attracted much interest in recent years [1]. These materials can be synthesized from bis(alkoxysilyl) precursors $(RO)_3Si\ R\ Si(OR)_3$ in the presence of surfactants acting as structure directing agents. By varying the organic linker group R, mesostructured materials tailored towards specific applications can be prepared. Recently, the synthesis of optically active PMO materials with interesting fluorescent properties [2] and hole conductivity [3] has been reported. The confinement of such materials within the pores of anodic alumina membranes could offer new features such as high aspect ratios of the pore system combined with high mechanical stability [4].

The synthesis of PMO materials confined within anodic alumina membranes (AAM) was based on the evaporation-induced self-assembly (EISA) process using siloxane precursors with biphenylene bridges. This type of precursor shows low solubility and a high hydrolysis rate leading to almost instant precipitation under common synthesis conditions. Here, by using an adapted EISA protocol, well-ordered mesostructures were successfully obtained with 4,4'-bis(triethoxysilyl)biphenyl (BTEBp, high fluorescence quantum yield) and three-armed oligo(phenylenevinylene)silane (3a-OPV, good hole conductivity) as precursors, respectively. The structure of the composite membranes was studied by small angle X-ray scattering (SAXS) in combination with transmission electron microscopy (TEM).

TEM micrographs show the formation of 2d-hexagonal circular and cubic mesophases for the BTEBp system. In the case of 3a-OPV system, circular and cubic mesophases could also be obtained. We will also discuss the physical properties of these hierarchical nanostructured materials.

Acknowledgement: The authors thank the DFG (SFB 486), CeNS, NIM and CSC (China Scholarship Council) for supporting this work.

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## Single-Enzymes in Zero-Mode-Waveguides and Nanopositioned Designer-Networks

**Stephan Heucke, M. Strackharn, S. Stahl, E. Puchner*, G. Acuna, P. Tinnefeld, H. E. Gaub**

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** now at: Lim-Lab, University of California, San Francisco*

Single-enzyme experiments give great insights into cell biology while also advancing medical research. We are currently pushing forward two new techniques that overcome limitations common in the field - thus enabling in vitro single-enzyme experiments at more natural conditions:

Zero-Mode-Waveguides (ZMWs) are cover slips with a nanoporous aluminum-coating. They reduce the observation volume in confocal microscopy by a factor of 1000. This enables optical single-enzyme experiments (e.g. FCS) with labeled substrate concentrations at the natural millimolar regime. Combined with our AFM force pulling techniques ZMWs also give the opportunity to optically observe substrate binding in force-activated enzymes such as titin kinase.

In order to design enzyme networks we use a novel bottom-up assembly method named Single-Molecule Cut-and-Paste (SMCP). Here single-molecules are picked up from a depot and positioned in a previously empty target area with an AFM tip and the help of differentially coupled force anchors. Thus SMCP provides the ability to isolate single enzymes at designated positions with nanometer precision. A surface of charged supported lipid bilayer prevents diffusion of the DNA-substrate into the bulk mimicking natural compartmentation. With these networks we want to be able to study enzyme interaction at a single-molecule level.

## Living cell interactions with micro-structured environments

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Cellular function is triggered by intracellular signalling cascades on small temporal and spatial scales. One prime example is cell migration, a process which is induced by actin polymerization that reorganizes the cytoskeleton, e.g. creating protrusion forces. Cell migration reflects the cellular micro-architecture and is a response to external stimuli, including the mechanical properties of the environment.

We investigate interactions of D. discoideum cells with periodically structured, three dimensional micro-environments. Our focus is set on the intracellular actin distribution as a reaction to the structured sample and on a resulting directionality of the migration, caused by cellular actin polymerization waves propagation aligned to the structure.

## Imaging and growth of carbon nanotubes

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Semiconducting single-walled carbon nanotubes are one-dimensional photoactive quantum systems with the potential for novel optoelectronic nanoscale applications such as light-emitting diodes or high sensitivity near-infrared detectors. Studies of optical properties of semiconducting nanotubes have emerged recently with ensemble experiments. Subsequent improvement of measurement sensitivity down to the level of individual nanotubes has triggered further progress in the understanding of the photophysical phenomena.

We focus our studies on individual carbon nanotubes. Our results group into two main achievements: firstly, we succeeded to establish complementary imaging techniques based on cryogenic photoluminescence, scanning electron microscopy and atomic force microscopy imaging of sample regions with separated single nanotubes. Systematic characterization methods allow us now to deterministically fabricate samples with individual nanotubes dispersed on substrates for optical spectroscopy at low-temperatures down to 4.2 K. Secondly, we have made progress in nanotube growth using a home-built methane chemical vapour deposition setup. Our efforts are directed towards diameter selective growth of suspended ultra-clean carbon nanotubes which would allow us to study intrinsic photophysics of one-dimensional systems unmasked by defects or environmental fluctuations.

## A unified gas model of nucleosome positioning

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Within the last few years, genome-wide maps of nucleosome positions in different eukaryotes have revealed a salient pattern around transcription start sites, involving a nucleosome-free region (NFR) flanked by a pronounced periodic pattern in the average nucleosome density. A number of recent theoretical studies have focused on this periodic pattern  in S. cerevisiae and established a one-dimensional hard-core gas model as a successful null-model to describe this pattern. We compare the nucleosome organization downstream of NFRs in 12 *Saccharomycotina* yeast species. We find statistical positioning to describe nucleosome organization; but the simple hard-core gas model needs to be extended: The quantitatively different patterns can all be described within a unified one-dimensional gas model which takes nucleosome's internal degrees of freedom (i.e., transient unwrapping) into account. To explain the difference between the species' nucleosome patterns it suffices to assume a nucleosome density which varies among species while the other parameters describing the nucleosome's internal degrees of freedom are equal among species. The yeast *K. lactis* presents an anomolous feature; here we observe an increased effective width of nucleosomes, which we hypothesize is due to the linker histone H1.

## High Resolution Optical Tweezers for Single Molecule Studies of Eukaryotic Transcription

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Investigating mechanical aspects of single RNA polymerases will further our understanding of the molecular mechanism of transcription elongation. For these single molecule experiments we establish a high resolution optical tweezers setup in the dual trap design, where one trap is maneuverable by a piezo-driven mirror. Experiments with 5 kbp DNA tethers attached to trapped beads have shown that our current resolution is about 0.5 nm for forces measured around 15 pN at a time resolution of approximately 0.1s. This is sufficient to study single base pair steps of RNA Polymerase II on DNA. In further experiments we will investigate the behavior of RNA Polymerases I and II from a mechanical perspective. In addition, we will study transcription regulation by performing experiments in presence of different transcription factors such as TFIIS and TFIIF.

## On Superradiant Phase Transitions in Circuit QED

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Circuit QED systems of artificial atoms interacting with microwaves have been proved to behave in many respects analogously to their counterparts with real atoms in cavity QED. However, it has been predicted recently that the analogy fails if a large number of (artificial) atoms couple strongly to the electromagetic radiation [1]: Whereas for real atoms no-go theorems rule out the possibility of a superradiant quantum phase transition as the coupling is increased [2], the standard description of circuit QED systems in terms of macroscopic quantities [1,3] does allow it.

We investigate the possibility of a superradiant quantum phase transition in circuit QED systems from a microscopic point of view. Our analysis challenges the applicability of the standard description of circuit QED systems in the regime under concern and indicates even a qualitative deviation from its prediction.

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## A DNA Origami Framework for the Study of Single Molecule Conformational Dynamics

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Protein conformational changes play a critical role in cellular processes such as motility and signaling. Typical dimensions of cellular components are on the order of a few nanometers and their diverse cellular functions often involve movements ranging from fractions of a nanometer up to tens of nanometers. The current state of the art tool for studying conformational dynamics is single molecule Fluorescence Resonance Energy Transfer (FRET), whereby energy transfer between two fluorescent dyes is correlated to their spatial separation; however, several challenges limit the applicability of FRET for quantifying conformational dynamics. For example, distance predictions made by FRET theory are only accurate in the near vicinity of the FRET dye pair Förster radius, $R_0$ (3-7 nm), which depends on the spectral overlap of the dyes. $R_0$ itself is often difficult to determine owing to uncertainties in the relative orientation of donor and acceptor dipoles, thus making it difficult to conduct quantitative distance and displacement measurements with FRET. Here we present a nanoscale device resembling a nanoscale tweezers constructed from DNA origami that integrates nanostructures built from self-assembled DNA, attachment sites for molecules of interest, sites for surface immobilization, and fluorescent markers for the direct visualization of biomolecular dimensions and dynamics. Our nanoscale sensor provides a framework to both improve the quantitative accuracy and extend the scope of FRET-measurements. For the purpose of proof-of-concept studies we specifically integrated a piece of double stranded DNA (dsDNA) containing a recognition sequence for Catabolite Activator Protein (CAP), which is know to bend dsDNA upon binding, between the arms of this device. The bending angle will be evaluated with single particle electron microscopy (EM), and FRET microscopy will be employed in solution to resolve real-time kinetics and deformations of CAP-DNA binding.

## Analysis and manipulation of Dicer activity in a force-based assay

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Understanding protein translation is essential for the development of new and more successful therapies against major illnesses like cancer or HIV. One regulatory element of protein translation is the endoribonuclease Dicer that cuts double-stranded RNA independent of the sequence into pieces of 19-22 base pairs starting the RNA interference pathway and activating miRNAs. With the Molecular Force Assay (MFA) developed in our lab, we analyze the activity of Dicer with dsRNA and, especially, the possibility to hinder Dicer from cutting, thus creating a toehold for influencing protein translation.

The MFA is a highly parallel technique on the single-molecule level that, in contrast to the AFM, compares molecular bonds against each other. Two molecular complexes, a sample and a reference bond, are linked in series in the zipper mode between two surfaces. Upon retraction of the upper surface a force is loaded on the whole construct until the weaker of the two complexes ruptures. A fluorophore attached to the linker between the two bonds identifies the stronger, intact complex so that a simple fluorescence read-out indicates the outcome of the experiment. This setup is very sensitive to small changes in structural stability and is, therefore, a very good tool for analyzing the interaction of ligands with their target sequences.

For the analysis of Dicer, a 38 bp dsRNA strand including a specific binding site for the aminoglycoside paromomycin (sample bond) is tested against a 21 bp dsDNA-strand (reference bond). Dicer slices only RNA and reduces the sample bond to around 18 bp, lowering the survival probability of the RNA complex. Thus, Dicer activity is detected. Addition of the specific ligand paromomycin hinders Dicer from binding to its target and stabilizes the sample bond so that the interaction of paromomycin with its binding sequence is quantified as well.

Summarizing, the MFA is an adequate tool for the detection of Dicer activity that can be blocked by RNA-binding molecules.

## Folding of Single Calmodulin Molecules Observed with Optical Tweezers

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The advent of Optical Tweezers in Single Molecule Force Spectroscopy allows for sub-nanometer resolution in the determination of equilibrium fluctuations. We use a dual beam high resolution setup to investigate the equilibrium fluctuations of single molecules of the eukaryotic calcium-dependent signal transducer calmodulin over several minutes.

The increased resolution over AFM experiments allows us to identify a multi-state folding scheme with several transitions. As opposed to the previously assumed independence of the N and C-terminal domain we observe enhanced folding and unfolding kinetics of a part of one domain in the presence of a folded neighboring counterpart. Our data suggest that despite the spatial separa-tion of the N and C domain there is measurable influence of the folding kinetics between the do-mains. We hypothesize that the folding of a single EF-hand of one domain depends on the presence of its folded complement domain.

## Approaching Quantitative Confocal Raman Spectroscopy – Micro-Phase Analysis and Zoning of Crystals

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Micro-phase identification and lateral chemical mapping can be obtained by confocal Raman spectroscopy in a straightforward manner due to the high sensitivity of Raman active vibrations towards chemical composition. However, quantitative interpretation of Raman data is a highly demanding task, since signal intensity is influenced by various factors such as environmental conditions, optical alignment, or choice of reference materials.

An approach to improve the efficiency of dye-sensitized solar cells is to create thin hybrid films of covalently linked $CN_x$-polymers on $TiO_2$ nano-crystals. Here, the crystallinity as well as the phase-purity (anatase/rutile ratio) of the samples are important for understanding their photoactivity. In order to assess these parameters also confocal Raman spectroscopy was employed.

In order to demonstrate the capability of quantitative analysis by Raman spectroscopy, we investigated both the prospects of trapping of highly toxic hexavalent $Cr^{6+}$ in non-toxic calcite crystals as well as the cross-sectional chemical composition of tourmaline minerals. Tourmaline minerals are important geochemical carriers of boron and they allow substitution of trace elements. The compositional variations give rise to colored bands which have a potential to be exploited as indicators of geochemical processes. Therefore, Raman results were calibrated with data from electron microprobe analysis.

## Actin nucleation and polymerization investigated using fluorescence fluctuation spectroscopy

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Actin filaments are cytoskeletal polymers that are fundamental for several biological processes including cellular motility, cytokinesis, and mechanical resistance. The nucleation mechanism, i.e. the formation of the stable tetramer via dimers and trimers, whether for spontaneous or assisted nucleation (e.g. via formin or ARP2/3) has been inferred mainly on the basis of kinetic modeling fitting only polymer measurements (i.e. pyrene fluorescence assays).

Fluorescence fluctuation spectroscopy is a technique that allows determination of the diverse fluorescence species and their dynamics. By following polymerization over 12 hrs, we observed the simultaneous decrease in monomer concentration with the concomitant appearance of polymer. Both parameters are used to determine a more reliable kinetic mechanism. Moreover, the decrease of monomer to a steady state indicates the critical concentration for the conditions used. Using this approach, we tested the influence of phalloidin, pH and actin concentration on the nucleation and polymerization processes. This is the first direct experimental evidence of the spontaneous nucleation mechanism, which is not only applicable for actin but also a general method to investigate any protein that undergoes polymerization or aggregation.

## Stimulated Emission Depletion Microscopy

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Stimulated emission depletion microscopy has been used to overcome the diffraction limit of normal confocal fluorescence microscopy and structures down to 19 nm in x and y have been resolved [1]. While for a long time the application of STED microscopy has been hindered due to the necessity of using complicated laser systems, the recent development of commercially available supercontinuum lasers have significantly lowered the cost and complexity of operating such a setup in a lab environment [2]. Here we present our current STED microscope setup using the aforementioned compact laser source. In conjunction with a highspeed-scanning stage this will allow for observing dynamic processes in vivo with nanoscale resolution. Restrictions in scanning speed are set by the repetition rate of the laser source (1 MHz at the moment) but are thought to improve as the demand for fast, high power supercontinuum lasers rises. We will discuss general design considerations for building a STED system as well as our recent advances in two-color STED microscopy.

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## Caught in Transition: Single Molecule Measurements of Protelomerase TelK-DNA Complexes

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Protelomerase TelK is a single-turnover protein responsible for forming DNA hairpins in linear prokaryotic DNA. As with many sequence-specific DNA-binding proteins (SSDBP), the mechanism by which TelK recognizes its target sequence to form DNA hairpins quickly and accurately is poorly understood. Here, we used a combination of single-molecule approaches to decipher this protein's mechanism.

Total internal reflection fluorescence microscopy (TIRFM) was used to visualize quantum dot labeled TelK protein interactions with DNA lacking the recognition sequence (figure 1). To date, SSDBPs imaged with TIRFM have been shown to undergo 1D DNA scanning as their primary method for finding DNA recognition sequences. We have found that TelK does undergo 1D diffusion as a monomer at low concentrations. However, TelK does not diffuse on the DNA at high TelK concentrations, instead forming immobile protein aggregates of multiple TelK monomers.

High resolution optical trap studies have shown that, surprisingly, TelK condenses nonspecific DNA at high concentrations, contrary to the currently accepted model for SSDBP search mechanisms (2). These DNA distortions are likely to correspond to the DNA bending observed in the TelK-DNA crystal structure (figure 2). The TelK concentration dependence for both DNA condensation and 1D motion suggests a model whereby TelK searches for its target site while loosely bound to DNA as a monomer, and aggregates (into dimers, most likely) to perform its function of DNA hairpin formation. Moreover, these DNA distortions are energetically expensive, making this indiscriminate binding behavior surprising. TelK may use an indiscriminate tight binding mechanism as a form of potential energy storage for the eventual energy-expensive formation of DNA hairpins, particularly since it does so in the absence of an external energy cofactor. These attributes may also be general characteristics of single-turnover proteins, which have yet to be well studied at the single-molecule level.

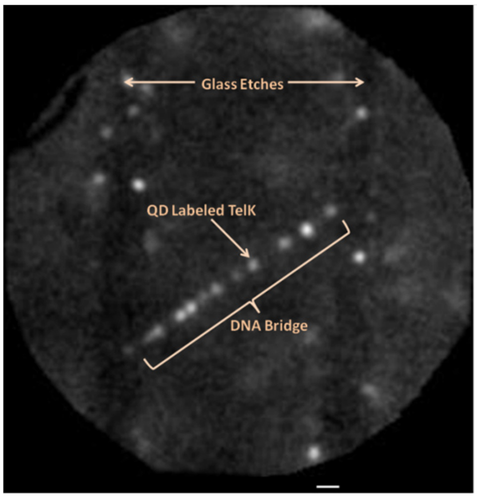

Figure 1. Quantum dot-labeled TelK on lambda DNA bridges visualized with TIRFM.

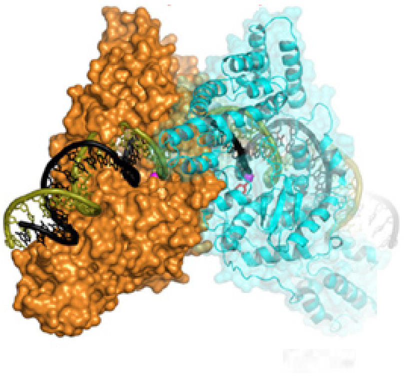

Figure 2. TelK complexed with DNA at the target site (1)

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## Structure and Dynamic of Hsp90 investigated by smFRET

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Hsp90 is a molecular chaperone required for survival of the cell under physiological conditions and during heat shock and for the activation of a large set of client proteins. It consists of two monomeric chains with dimerization interfaces at the C and N-terminal end [1].

The crystal structure of the completely (N- and C-terminal) closed state has been solved [1], but both the C- and N-terminal open states have not been crystallized yet. We use PIE-FRET to triangulate the position of these domains in the open state.

In addition, we investigate the N- and C-terminal dimerization kinetics of Hsp90 with smFRET [2,3]. Surprisingly, we find nucleotide dependent C-terminal dissociation / association kinetics on the timescale of seconds although the nucleotide binding pocket is far away in the N-terminal domain. Above that, N- and C-terminal opening and closing are anti-correlated. These findings are confirmed by well defined mutations [3].

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# Hotels

**DOMUS CILIOTA**

*Calle delle Muneghe - S. Marco, 2976*
*Tel: +39.041.5204888 - Fax: +39.041.5212730*
*http://www.ciliota.it, info@ciliota.it*

**Directions from hotel to workshop location:**
*Walk to the boat stop "S. Zaccaria" (~ 15 min) or take boat No. 1 from "S. Angelo" to "S. Zaccaria" (~19 min, every 10 min) and take boat No. 20 to San Servolo (10 min).*

**CENTRO CULTURALE DON ORIONE ARTIGIANELLI**

*Rio Terra' Foscarini - Dorsoduro 909/a*
*Tel. +39 041.5224077 - Fax +39 041.5286214*
*www.donorione-venezia.it, info@donorione-venezia.it*

**Directions from hotel to workshop location:**
*Walk to the boat stop "S. Zaccaria" (~20 min) and take boat No. 20 to San Servolo.*
**OR**
*Take boat No. 2 (~15 min) or 51 (~7 min) from stop "Zattere" to "S. Zaccaria". Then take boat No. 20 to San Servolo.*

**FORESTERIA VALDESE DI VENEZIA**

*Castello 5170, Calle Lunga S. Maria Formosa*
*Tel +39 041.5286797 - fax +39 041.2416238*

*Opening hours reception desk: 8:30 am - 8:00 pm.*
*http://www.foresteriavenezia.it/uk*
*info@foresteriavenezia.it*

**Directions from hotel to workshop location:**
*Walk to the boat stop "S. Zaccaria" and take boat No. 20 to San Servolo (boat trip: 10 min).*

**L'ISTITUTO PROVINCIALE PER L'INFANZIA SANTA MARIA DELLA PIETÀ**

*Castello - Calle della Pietà 3701*
*Tel. +39 041.5222171 / .5237395 - Fax: +39 041.5204431*
*http://www.pietavenezia.org/casaferie.htm*
*info@pietavenezia.org*

**Directions from hotel to workshop location:**
*Walk to the boat stop "S. Zaccaria" and take boat No. 20 to San Servolo (boat trip: 10 min).*

# Timetables

**GROUP BUS TO VENICE AND BACK TO MUNICH**

| To Venice (19.09.) | | Back to Munich (24.09.) | |
|---|---|---|---|
| Munich (LMU Main building) | Venezia Piazzale Roma | Venezia Piazzale Roma | Munich (LMU Main building) |
| 10:00 | ~ 18:30 | 14:00 | ~ 22:30 |

**BOAT LINE 20 TO WORKSHOP LOCATION (SAN SERVOLO)**

| To San Servolo | | Back to Venice | |
|---|---|---|---|
| S. Zaccaria | S. Servolo | S. Servolo | S. Zaccaria |
| 6:55 | 7:05 | 8:35 | 8:45 |
| 7:15 | 7:25 | 8:45 | 8:55 |
| 8:15 | 8:25 | 9:10 | 9:20 |
| 8:35 | 8:45 | 9:40 | 9:50 |
| 9:00 | 9:10 | 10:00 | 10:10 |
| 9:20 | 9:30 | 10:50 | 11:00 |
| 9:50 | 10:00 | 11:20 | 11:30 |
| 10:30 | 10:40 | 12:10 | 12:20 |
| 11:10 | 11:20 | 12:40 | 12:50 |
| 11:50 | 12:00 | 13:30 | 13:40 |
| 12:30 | 12:40 | 14:00 | 14:10 |
| 13:10 | 13:20 | 14:50 | 15:00 |
| 13:50 | 14:00 | 15:30 | 15:40 |
| 14:30 | 14:40 | 16:00 | 16:10 |
| 15:10 | 15:20 | 16:50 | 17:00 |
| 15:50 | 16:00 | 17:30 | 17:40 |
| every 40 min until | | 18:00 | 18:10 |
| | | 18:50 | 19:00 |
| | | 19:20 | 19:30 |
| 20:30 | 20:40 | 20:10 | 20:20 |
| every hour until | | 20:40 | 20:50 |
| 1:30 | 1:40 | 21:50 | 22:00 |

# Internet

Two PC rooms with internet connection are accessible for the participants are located next to the conference hall. Please ask for the keys and login in the conference office next to the lecture hall.

Access to the WLAN internet will probably be available in the lecture hall. Information will be provided at the conference.


Valdese
Pieta
Ciliota
Don Orione
CANAL GRANDE
BACINO DI SAN MARCO
CANALE DELLA GIUDECCA
GIUDECCA
PIAZZA SAN MARCO
Basilica di San Marco
Palazzo Ducale
Ponte di Rialto
Santa Maria della Salute
Gallerie dell'Accademia
Collezione Peggy Guggenheim
Teatro la Fenice
S. Maria d. Frari
Chiesa di San Giorgio Maggiore
Ospedale Civile
Stazione Marittima

# NOTES

# NOTES

# CeNS Workshop 2010: Nanosciences – Merging Disciplines / Venice International University, San Servolo (Italy) / September 20 – 24, 2010

| Time | Monday, September 20th | Tuesday, September 21st | Wednesday, September 22nd | Thursday, September 23rd | Friday, September 24th | Time |
|---|---|---|---|---|---|---|
| **9:00** | *Boat departing at 9:00* | *Boat departing at 9:00* | *Boat departing at 9:00* | *Boat departing at 9:00* | *Boat departing at 9:00* | **9:00** |
| 9:20 | **Mildred S. Dresselhaus** | **Laurens (Kobus) Kuipers** | **Don Lamb** | **Edward A. Bayer** | **Claudia Veigel** | 9:20 |
|  | The Promise of Nano-Materials for Energy Related Applications | Nanoscale light control | Aging and Viruses: What single molecules reveal about the Nemeses of Life | Designer cellulosomes as a viable macromolecular platform for the nanosciences | Basic mechanism of myosin motors studied at the single molecule level |  |
| 10:05 | **Lukas Schmidt-Mende** | **Andrey A. Lutich** | **Zan Luthey-Schulten** | **Tim Liedl** | **Uwe Bunz** | 10:05 |
|  | Nanostructured Organic and Hybrid Solar Cells | Optical manipulation of gold nanoparticles: from basics to applications | Molecular and cellular studies of dynamical networks in translation | DNA Origami and DNA Tensegrity | Conjugated Polymers of the PPE type and their Gold Nanoparticle Complexes |  |
| **10:50** | ***Coffee break*** | ***Coffee break*** | ***Coffee break*** | ***Coffee break*** | ***Coffee break*** | **10:50** |
| 11:15 | **Kostya S. Novoselov** | **Ben Feringa** | **Ulrich Schollwöck** | **Xiang Zhang** | **Michel Brune** | 11:15 |
|  | Materials in the Flatland | In Control of Molecular Assembly & Motion | Relaxation dynamics in finite closed quantum systems | Optical Meta Materials and Nano Plasmonics | Quantum theory of measurement at work by photon counting in a box |  |
| **12:00** | ***Lunch*** | ***Lunch*** | ***Lunch*** | ***Lunch*** | **Departure:**<br>**Boat leaves at 12:10 and 12:40**<br>**Bus leaves at 14:00 from Piazzale Roma** | **12:00** |
| 14:30 | **Johan Hofkens** | **Nadia Ruthardt** | **Informal discussions** | **Jelena Vuckovic** |  | 14:30 |
|  | In situ monitoring of catalysis at the nanoscale | Live-cell imaging and single-particle tracking of polyplex internalization |  | Quantum dots in photonic crystals: from cavity QED to optical switches and quantum gates |  |  |
| 15:15 | **Christian Ochsenfeld** | **Ulrike Gaul** |  | **Achim Hartschuh** |  | 15:15 |
|  | Quantum-Chemical Calculation of Intermolecular Interactions for Molecular Systems with 1000 and More Atoms | Decoding regulatory gene networks – towards a systems biology of development |  | Enhancing and localizing light-matter interaction using optical antennas |  |  |
| **16:00** | ***Coffee break*** | ***Coffee break*** |  | ***Coffee break*** |  | **16:00** |
| 16:30 | **Teun M. Klapwijk** | **Klaus Müllen** |  | **Laurens Molenkamp** |  | 16:30 |
|  | Superconducting nano-sensors for THz radiation detection | Graphene as Unique Multitalent – Catalyst, Semiconductor, Nanowire, Protein Template |  | Dirac Fermions in HgTe Quantum Wells |  |  |
| 17:15 | **Leo P. Kouwenhoven** | **Short presentation of selected posters I** |  | **Short presentation of selected posters II** |  | 17:15 |
|  | Quantum Opto-Electronics with Semiconducting Nanowires and Carbon Nanotubes |  |  |  |  |  |
| 18:00<br>-<br>20:00 | **Welcome reception** | **Poster Session I** |  | **Poster Session II** |  | 18:00<br>-<br>20:00 |