

An aerial photograph of Kloster Seeon, a large island in the middle of Chiemsee. The island is surrounded by water and has several buildings with red roofs. The surrounding area is forested and hilly.

**Internal
CeNS-Workshop**

Keynote Topic:
“Transport in Nanosystems”

Kloster Seeon, Chiemsee

28.-30. September, 2003

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Scientific Coordinators:
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Internal Workshop of the  **CeNS**
Center for NanoScience
Ludwig-Maximilians-Universität

September 28 – 30, 2003

**Keynote Topic:
“Transport in Nanosystems”**

Program:

Sunday, September 28, 2003

8.00h	Departure of conference bus from Geschwister-Scholl-Platz 1 (University Main Building)
8.20h	Departure of conference bus from Munich Ostbahnhof (bus terminal)
9.45h	Arrival at Kloster Seeon; Klosterweg 1, 83370 Seeon
10.30h–12.00h	Registration
12.00h– 12.50h	<i>Lunch</i>
12.50h – 13.00h	Welcome
13.00h – 13.30h	Reinhard Guckenberger <i>High-resolution imaging of single fluorescent molecules with a new probe for scanning near-field optical microscopy</i>
13.30h – 14.00h	Daan Wouters <i>Probe lithography and chemical modification of nanometer-sized structures</i>
14.00h – 14.30h	Gunnar Raschke <i>A Single Gold Nanoparticle Sensor for Biomolecular Recognition</i>
14.30h – 15.00h	Alexander Högele <i>Spectroscopy on single self-assembled quantum dots</i>
15.00h – 15.30h	Nenad Ocelic <i>Infrared near-field microscopy of focused ion beam patterned SiC</i>
15.30h – 16.00h	<i>Coffee Break</i>
16.00h – 16.30h	Claudia Friedsam <i>Investigation and manipulation of single polyelectrolyte molecules adsorbed on solid supports by the use of an AFM</i>

16.30h – 17.00h	Ulrich Gerland <i>The use of nanopores for RNA structure determination</i>
17.00h – 17.30h	Marc Tornow <i>Controlled release of immobilized DNA into electrolyte solution</i>
17.30h – 18.00h	Schwaiger, Ingo <i>Single molecule mechanics of proteins</i>
18.00h – 18.30h	Christine Meyer <i>Nanotweezers - detection of their deflection</i>
18.30h – 19.00h	Elisabeth Lupton <i>Siloxane Elastomers under Tensile Stress: A First Principles Molecular Dynamics Study</i>
19.00h – 20.30h	<i>Dinner</i>
20.30h – 22.00h	Poster Session Group 1

Monday, September 29, 2003

7.30h – 9.00h	<i>Breakfast</i>
9.00h – 10.00h	<i>Keynote lecture:</i> Christoph Strunk <i>The current phase relation in proximity coupled Josephson junctions</i>
10.00h – 10.30h	Frank Wilhelm <i>Engineering quantum (de)coherence in superconducting devices</i>
10.30h – 11.00h	<i>Coffee Break</i>
11.00h – 12.00h	<i>Keynote lecture:</i> Thomas Palberg <i>Mobility and Charge Determination from Electrokinetic Experiments on Isolated Charged Colloidal Spheres, Colloidal Fluids and Crystals</i>
12.00h – 13.30h	<i>Lunch</i>
13.30h – 14.00h	Simon Keller <i>Dynamics of DNA measured by fluorescence correlation spectroscopy</i>
14.00h – 14.30h	Xaver Schlagberger <i>Dynamics of Driven Polymers</i>
14.30h – 15.00h	Friedrich Simmel <i>Experiments on DNA in electric fields</i>

15.00h – 15.30h	Wendy Huynh <i>Templating Nanostructures with DNA</i>
15.30h – 16.00h	<i>Coffee Break</i>
16.00h – 17.00h	<i>Keynote lecture:</i> Werner Kunz <i>Some aspects of modern electrolyte chemistry</i>
17.00h – 17.30h	Udo Beierlein <i>Driving current through organic molecules</i>
17.30h – 18.00h	Michael Sindel <i>Quantum dots coupled to polarized leads - NRG study</i>
18.00h – 19.00h	<i>Keynote lecture:</i> Yuval Oreg <i>Many body phenomena in artificial atoms</i>
19.00h – 20.30h	<i>Dinner</i>
20.30h – 22.00h	Poster Session Group 2

Tuesday, September 30, 2003

7.30h – 9.00h	<i>Breakfast</i>
9.00h – 9.30h	Eduardo Mendoza <i>Signal transport in the chemical compass of eucaryotic cells</i>
9.30h – 10.00h	Don C. Lamb <i>Single Molecule Studies of RNA Polymerase</i>
10.00h – 10.30h	Robert Stark <i>Transient forces in dynamic atomic force microscopy</i>
10.30h – 11.00h	<i>Coffee Break</i>
11.00h – 11.30h	Christian Hellriegel <i>Single Molecule Spectroscopy and Microscopy in Nanostructured Molecular Sieves</i>
11.30h – 12.00h	Lorenz Kampschulte <i>STM, TDS and LEED examinations of trimesic acid on single crystal surfaces</i>
12.00h – 12.10h	Closing remarks
12.00h – 13.30h	<i>Lunch</i>
15.00h	Departure of conference bus from Kloster Seeon Klosterweg 1, 83370 Seeon
16.25h	Arrival of conference bus at Munich Ostbahnhof (bus terminal)
16.45h	Arrival at Geschwister-Scholl-Platz 1 (University Main Building)

Lectures Abstracts

Driving current through organic molecules

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We report electronic transport measurements on gold/1,4-phenylene-diisocyanide/gold junctions using two different contact architectures. In the first technique, the self-assembled monolayer (SAM) of 1,4-phenylene diisocyanide is sandwiched between electron-beam defined bottom and top metallic contacts. The second architecture employs opposing planar gold contacts with a sub 10 nm gap between them, in which chains of 1,4-phenylene diisocyanide can be inserted. Low temperature measurements showed characteristic peak structures in the conductance curves as a function of source-drain voltage. These features may be attributed to either Coulomb blockade effects, coherent transport through the molecular eigenstates or to vibrational modes of the molecule.

Investigation and manipulation of single polyelectrolyte molecules adsorbed on solid supports by the use of an AFM

Claudia Friedsam, Markus Seitz, Hermann Gaub
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Center for NanoScience CeNS

AFM-based force spectroscopy is a powerful method that allows the measurement of intra- and intermolecular forces of single molecules. The molecular interactions investigated by this technique range from entropic forces in single polymer coils to the rupture forces of individual covalent bonds.

In particular, it is possible to investigate the desorption forces of single polymer chains from solid surfaces in solution, under equilibrium conditions. Previous desorption studies of polyvinylamines from equilibrated physisorbed polymer films on silica had shown that the Coulombic contribution to the interaction between polymer and substrate depends linearly on Debye screening length and the polyelectrolyte's line charge density.

The (additive) Non-Coulombic contribution to the desorption force reflects other binding interactions (van der Waals, coordinative bonds) between the polymers and the solid substrate. Also, intermolecular interactions between two or more polyelectrolyte molecules could be observed in the presence of divalent metal ions.

These measurements were now extended to other substrates, particularly gold, mica and calcite, and to negatively charged polyelectrolytes, such as polyacrylic acid and DNA. Hereby, appropriate chemical modification allowed for binding of a few individual polymer chains to the AFM tip, which is necessary for the investigation of repulsive Coulombic contributions and for the long-term study of the same molecules under various conditions.

Based on recent results, the reversible control of surface adhesion of individual polymer chains by the manipulating the surface potential of conducting (metal) substrates will be discussed.

The use of nanopores for RNA structure determination

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Since the discovery of catalytically active RNA molecules (ribozymes), the sequence-structure relationship and the folding mechanism of RNA has been of great interest to biochemists. Recently, physicists have introduced single-molecule manipulation techniques such as optical tweezers to the study of RNA folding. With these devices, one can exert and measure mechanical forces in the piconewton range on the ends of RNA molecules. This allows controlled 'unzipping' of RNA structure while recording precise positional information. We show that the experimental force-extension curve for a small RNA hairpin is well described by a theoretical model which includes the basepairing energetics of RNA and a freely jointed chain model for its polymer properties. We then extend this model to address the question of what can be learned by pulling on larger RNA molecules. In particular, we argue that useful structural information on RNA molecules, which is not obtainable by simple unzipping from the ends, can be obtained instead by mechanically pulling RNA through a nanopore, which allows single, but not double strands to pass. We demonstrate within an explicit theoretical model how RNA secondary structure, including pseudoknots, could be recovered from such measurements. RNA therefore emerges also as an ideal model system with which to study the characteristics and capabilities of single-molecule approaches, both experimentally and theoretically.

High-resolution imaging of single fluorescent molecules with a new probe for scanning near-field optical microscopy

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A new probe (1) for Scanning Near-field Optical Microscopy (SNOM) that exploits field concentration at a metal tip allows to image single dye molecules at a resolution far beyond the diffraction limit. This new probe combines the high resolution of the apertureless SNOM with the single molecule sensitivity of the aperture SNOM. We present optical images of single Cy-3 fluorophores covalently attached to the termini of DNA. The dyes appear as characteristic patterns with details of 10 nm in width. Modeling of the data allows determining the position of the dyes and also their 3-D orientation. As an important feature of the new probe, the metal tip simultaneously provides high-resolution topographic imaging. Thus the optical data can directly be correlated with structural information. With this unique combination of qualities the new probe promises exciting applications on biological samples.

- (1) H. G. Frey, F. Keilmann, A. Kriele, and R. Guckenberger, "Enhancing the resolution of scanning near-field optical microscopy by a metal tip grown on an aperture probe," *Appl. Phys. Lett.*, **81**, 5030-5032 (2002).

Single Molecule Spectroscopy and Microscopy in Nanostructured Molecular Sieves

C. Hellriegel*, J. Kirstein, C. Jung, C. Bräuchle
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About a decade ago the single molecule spectroscopy (SMS) was restricted to very special molecules and materials. Meanwhile a wealth of systems can be analysed using SMS, ranging from biological to inorganic systems.

Materials with structural properties on the scale length of nanometres such as molecular sieves pose ideal environments to incorporate single molecules in an ordered fashion. We have recently been able to demonstrate the possibility to detect single fluorescent dye molecules incorporated as guests in such materials by confocal microscopy. We gain additional information from the molecule by recording its emission spectra and by determining the molecule's orientation. In some cases we can directly observe the motion of molecules inside a porous network, the changing of their orientations and spectral shifts.

The characterisation of individual molecules, their nearest environment and the interactions between the molecules and their environment is a fundamental step towards the development of devices based on single molecules in nanoporous cages.

Spectroscopy on single self-assembled quantum dots

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Self-assembled semiconductor quantum dots are rather small objects with a height of a few nanometers and a few tens of nanometers in lateral dimensions. Hence, the motion of charge carriers -electrons or holes - trapped in the potential of a quantum dot exhibits quantisation in all three dimensions. Therefore quantum dots represent an ideal model system for the study of quantum mechanical properties of charged particles and their interactions.

The basic experimental approaches to the examination of quantum dots are the transport and the optical spectroscopy techniques. Here, we focus on the photoluminescence spectroscopy and the newly developed absorption spectroscopy performed on single self-assembled quantum dots. Neutral and charged electron-hole pairs (excitons) localised within a single quantum dot are probed through interaction with coherent laser light. Among the addressed aspects are the lifetime of the excitonic ground state, the transition electric dipole moment and the fine structure splitting due to spin mediated electron-hole interaction.

Templating Nanostructures with DNA

Wendy Huynh
Ludwig Maximilians Universität München
Center for NanoScience CeNS

Because of its self-assembly properties, the biological molecule DNA been recently considered for application in electronic devices and sensors. The base-pairing specificity of DNA permit the molecule to be positioned on the nanoscale at electrodes and on surfaces where the complementary bases can be found using simple, solution-based, processing methods. After much debate however, it appears that DNA is a largely insulating material and cannot on its own be considered as an active component of electronic devices. We can nevertheless, combine the unique self-assembly properties of DNA with metallic or semiconducting behavior by directly growing metals or semiconductors on this biological molecule. In this talk the results of stretching and aligning DNA between electrodes as well as of its use as a template for growth of II-VI semiconductors and organic and inorganic metals will be presented. We find that DNA templates the growth of 1-5 nm diameter nanoparticles that assemble in a beads-on-a-string manner. In some cases, the nanoparticles can be assembled such that they form a current conducting pathway.

STM, TDS and LEED examinations of trimesic acid on single crystal surfaces

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The adsorption of trimesic acid (TMA) on single crystal surfaces was studied by STM (Scanning Tunnelling Microscopy), TDS (Thermal Desorption Spectroscopy) and LEED (Low Energy Electron Diffraction). Trimesic acid consists of a benzene ring with three carboxylic groups in symmetric 1,3,5-positions. Three different single crystals were used as substrates: graphite(0001), silver(111) and gold(111).

The measurements were done under Ultra High Vacuum (UHV) and also ambient conditions. In UHV trimesic acid was evaporated on different substrates using an effusion cell. In ambient conditions the TMA molecules were measured at the liquid-solid interface. The preparation of a TMA monolayer under UHV conditions was observed and adjusted with thermal desorption spectroscopy. From these measurements it was possible to deduce the binding conditions. In all cases characteristic periodically arranged structures could be demonstrated. In the monolayer regime the structure is characterized by non-dense-packing of molecules on the surface. It was shown that, depending on the substrate material and the preparation method, different network structures could be assembled. These networks are induced by directed hydrogen bonding (self assembly), forcing the organic molecules to build a two-dimensional grid architecture with small cavities.

Another point of interest was filling these cavities with guest molecules. Besides TMA, several other molecules could be inserted, e.g. buckyballs (C_{60}) and ligand stabilized gold clusters ($Au_{55}(PPh_3)_{12}Cl_6$).

For these experiments it is useful to have an ambient condition STM and an UHV STM side by side. The ambient condition STM allows simple sample preparation and handling, while the UHV STM offers high-resolution imaging and cooling possibilities.

Dynamics of DNA measured by fluorescence correlation spectroscopy

Simon Keller
Ludwig Maximilians Universität München
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The technique of fluorescence correlation spectroscopy (FCS) has become an important tool for investigating the properties of single molecules in solution. Fluorescently labelled particles diffusing through a small and fixed volume element formed by a laser focus will undergo excitation and emit light, that is collected into an avalanche photodiode. A time-correlation analysis of the fluctuations in the detected intensity yields quantities as diverse as diffusive behaviour, reaction kinetics or local particle concentrations.

We applied the method to polymeric model systems like DNA. Variation of the chromophore number density along the contour of a single λ -phage DNA (~16 μ m length) leads to different values in the measured diffusion parameters. The reason for these differences are internal chain relaxations, which show length scale dependent dynamics.

Further, the dependence of the diffusion properties on polymer concentration was investigated.

Some aspects of modern electrolyte chemistry

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Electrolytes, i.e. salts composed of small ions are ubiquitous in nature and industry. Their properties are widely investigated since the 19th century, mainly because of the precise conductivity measurements, which could be carried out already at that time. The theory of Debye and Hückel was a first summit of statistical mechanics, and in many respects the Debye-Hückel (DH) theory is still the reference point for any further description of electrolytes.

In the last century the description of electrolytes in simple liquids was well developed so that today the structure of liquid salt solutions can well be modelled with computer simulations and integral equation theories. In the first part of this paper a survey of the main results and the strategies to describe these systems will be given, both for structural and thermodynamic properties and for transport properties (diffusion and conductivity).

In industry electrolytes are often additives to complex solutions. In this case all the rigorous statistical mechanical approaches appear to be much too complex. As a result engineers still use simple extensions of the DH theory with considerable numbers of adjustable parameters. Surprisingly, the modern fitting procedures have also a predictive character. Some examples will be shown in the second part of the paper.

Finally, electrolytes play an important role in biology and colloidal chemistry. Here the situation is similar to industry. Only very rough models are commonly used for ions near surfaces. Apart from the charges only the size of the radii is considered, if at all. Therefore many specific ion effects remain unexplained or they are only qualitatively described in terms of "hard" and "soft" ions, "structure-maker" and "structure breaker" etc. Some new ideas to include ion specificity in colloidal and biological systems are presented in the third part of this paper, both from an experimental and a theoretical point of view.

Single Molecule Studies of RNA Polymerase

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RNA polymerase (RNAP) transcribes the genetic information in a template DNA strand into a complementary RNA strand. Transcription is the first step in gene expression and is the target of many regulation mechanisms within the cell. To investigate the structure and function of RNAP, we have performed fluorescence resonance energy transfer (FRET) measurements on single molecules. Fluorescent markers were placed at different locations along the DNA strand and the FRET pair was attached to the 5' end of the RNA. Measurements were performed on complexes constructed using either DNA with an 'artificial bubble' (a region containing 9 mismatched base pairs) and an 8-mer RNA primer or using DNA containing the *E. Coli* A1 promoter site from the T7 bacteriophage. The distribution in energy transfer efficiency of the different labeling positions were investigated both before and after addition of nucleotides.

Siloxane Elastomers under Tensile Stress: A First Principles Molecular Dynamics Study

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Center for NanoScience CeNS

The unique properties of siloxane elastomers result in their application as sealants and adhesives where resistance to tear is crucial. The understanding of elastic properties of single molecules has now been made possible with the development of AFM for stretching of single molecules. In order to interpret the results of AFM experiments to be performed on single siloxane polymers and to provide insight into the tear process at a molecular level we have performed Car-Parrinello molecular dynamics (CPMD) calculations to characterize the response of siloxane elastomers to tensile stress. CPMD provides a computationally efficient approach to examine mechanically induced reactions at the ab-initio level [1,2].

We present results on the siloxane dimer, trimer and hexamer under different loading rates. Our results include bond rupture forces and a mechanism for the bond breaking process. Future work will focus on determining the influence of solvent molecules, the anchoring of the molecule to the substrate and the AFM tip and determining a mechanism for crack propagation in the bulk material.

References:

1. D. Aktah, I. Frank; J.Am.Chem.Soc. 124, 3402, 2002.
2. U.F. Rvhrig, I. Frank; J.Chem.Phys. 115, 8670, 2001.

Signal transport in the chemical compass of eucaryotic cells

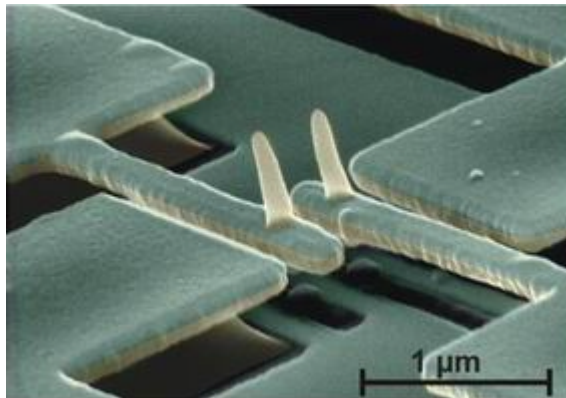
E. Mendoza
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Many biological systems have the ability to sense the direction of external chemical sources and respond by polarizing and migrating toward chemoattractants or away from chemorepellants. This phenomenon, referred to as chemotaxis, is crucial for the proper functioning of single-cell organisms, such as bacteria and amoebae, and multi-cellular systems as complex as the immune and nervous systems. Bacterial ("prokaryotic") chemotaxis has been successfully modelled over the last few years (work by Barkai, Leibler & collaborators, 1997-2001). The talk will discuss attempts at modelling the more complex and (very open) case of eukaryotic chemotaxis (eukaryotic = cell with a nucleus), in particular the initial gradient sensing function (which Weiner calls "the chemical compass") using diffusion (Levchenko-Iglesias, Biophysical Journal, Jan 02) and alternatively compartmentalized generalized mass action (cGMA) approaches (Bretschneider-Mendoza, work in progress).

Nanotweezers – detection of their deflection

Christine Meyer, Heribert Lorenz, and Khaled Karrai
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Center for NanoScience CeNS

Nano-Electromechanical Systems (NEMS) offer a wide range of applications in electronic as well as actuator devices. The detection of their nanoscaled deflection is therefore an extremely important task. We investigate silicon tweezers consisting of free standing nanometer-sized prongs. A bias voltage applied across the prongs leads to a deflection due to electrostatic forces.



We tested the functionality of our nanotweezers devices with a non-invasive optical technique. For this purpose, the tweezers were imaged with a home built scanning confocal microscope. A quasi-static low frequency ac excitation of the system was then identified in the reflected signal by demodulating it at the actuation frequency as well as at its higher harmonics. Even though the resolution of the confocal microscope in scanning mode is much less than the size of the nanostructure under investigation, the position of the tweezers can be determined from their rough silhouettes. By comparison of the scanning confocal image with the image of the demodulated signal, the mechanically actuating parts of the system can thus be identified. By this method, we are able to detect deflection amplitudes in the Angstrom range. This is a low cost and simple approach to reveal disfunctions of a device under test.

Infrared near-field microscopy of focused ion beam patterned SiC

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Silicon carbide was subject to investigations in various scientific and technical fields for many years. It turned out that, e.g., some features of stellar spectra could be ascribed to phonon-polariton resonances of small SiC grains, and that the outstanding electronic properties of SiC make it a promising material for high-power semiconductor devices.

Here we demonstrate the use of a home-built scattering-type (or apertureless) scanning near-field infrared microscope (s-SNIM) to study the local infrared properties of a SiC surface patterned by focused ion beam implantation. In our experiment the sharp probing tip of the microscope is illuminated by infrared light from a CO₂ laser and both the amplitude and phase of backscattered light are detected.

Tuning the laser between 10.6 μ m and 11.2 μ m, we find phonon-polariton resonance of the tip-sample near-field interaction[1] whose magnitude and spectral position strongly depend on the sample's local crystal structure. This enables us to differentiate between crystalline SiC and amorphous SiC regions produced by implantation, as well as the transition regions between them. Thus, our method could be used to map radiation damage caused by implantation process employed for semiconductor doping or to study crystal defects in thin film growth.

[1] R.Hillenbrand, T.Taubner, F.Keilmann, Nature, 418, 159-162 (2002)

Many Body Phenomena in Artificial Atoms

Yuval Oreg
Weizmann Institute of Science, Israel

Artificial atoms are small metallic particles in the nanometer scale. In this talk I will discuss recent theoretical and experimental developments concerning the role of spin and electron-electron interactions in artificial atoms. In contrast to natural atoms, it is possible to connect artificial atoms to electric reservoirs, and pass current through them. We will show that an appropriate tuning of the artificial atom parameters may form novel collective phenomena - belonging to a class of phenomena known as "the multi-channel Kondo effect". The latter can not be comprehended within the current paradigm theory of condensed matter metals (the so-called "Fermi-liquid theory"). The suggested structure of artificial atoms forms a new playground allowing both experimenters and theorists to explore in detail the nature of this type of many-body collective phenomenon.

Mobility and Charge Determination from Electrokinetic Experiments on Isolated Charged Colloidal Spheres, Colloidal Fluids and Crystals

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A charged particle subjected to an electric field E will acquire a constant velocity v due to the balance of accelerating electrostatic forces and friction forces. Within the standard electrokinetic model the mobility $\mu = v/E$ depends on the surface or Zeta-potential and thus on the particle charge. In this talk we present instrumental solutions to accurately measure μ at different particle concentrations ranging from Optical Tweezing Electrophoresis for isolated particles to integral flow measurements with Doppler Velocimetry for crystalline suspensions. The rich flow scenario observed there is presented in some detail. A prescription to determine the true mobility in the presence of additional friction between colloidal solid and cell wall is given. For isolated spheres on the other hand we observe the mobility to be independent of particle size and much lower than in the crystalline state. The latter findings are discussed in terms of an effective or renormalized charge.

A Single Gold Nanoparticle Sensor for Biomolecular Recognition

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K. Kürzinger and A. Nichtl

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We present a new optical biosensor based on scattering spectroscopy of *single* functionalized gold nanoparticles for the optical detection of molecular binding events.

The scattering spectrum of a noble metal nanoparticle is dominated by a collective oscillation of its conduction band electrons. The spectral position of this nanoparticle plasmon resonance (NPPR) is strongly influenced by the dielectric properties of the particle's immediate surrounding. Molecular binding events inside this nanoenvironment alter the refractive index and can therefore be deduced from a shifted resonance position. We monitor the *homogenous* NPPR spectrum of a single gold nanoparticle which allows us to detect spectral shifts of only a few meV. Therefore, less than 100 molecules with a molecular weight of only 50 000 D can be detected under physiological conditions. We demonstrate the concept using gold nanoparticles functionalized with biotin to detect streptavidin molecules [1].

Apart from being sensitive to only 100 analyte molecules, single nanoparticle assays feature the possibility of miniaturization and hence massive parallelization.

[1] G. Raschke et al., Nano Letters, **3**, 935 (2003).

Dynamics of Driven Polymers

Xaver Schlagberger, Roland R. Netz
Ludwig Maximilians Universität München
Center for NanoScience CeNS

We investigate, using Brownian Dynamics simulations and scaling arguments, a semiflexible bead-spring chain as a model for a neutral or charged polymer in solution under the influence of an external field. In the latter case we explicitly add counterions. Hydrodynamic interactions are included via an approximate mobility tensor (Oseen or Rotne-Prager). The external field may be electrostatic or gravitational. We try to estimate the effect of coupling between hydrodynamic and elastic interactions. It is seen that for sufficiently stiff chains the orientation of the long axis of the polymer with respect to the external field direction depends on the relation of the stretching modulus to the bending modulus. We extrapolate the results to experimentally accessible regions (sedimentation and birefringence experiments). In the case of charged polymers polarization effects will overwhelm the hydrodynamic orientation.

Single Molecule Mechanics of Proteins

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Proteins are the most important class of biomolecules. The problem of how proteins fold into complicated 3D structure is still a challenge for both experimentalists and theorists. We have used Single Molecule Force Spectroscopy to investigate the folding of two proteins with different topological complexity. The coiled-coil is a simple structural motif which is involved in many important processes in cells. Force elongation curves of myosin II coiled-coil revealed a massive structural transition at forces between 20 and 25 pN where the coil extends to about 2.5 times its original length. An analysis based on an elastically coupled two-level system suggests the observed conformational change is an unfolding/folding transition. This transition is reversible on a sub-second timescale which shows that coiled-coil structures can produce significant mechanical force during folding. In contrast to coiled-coils the Ig fold of proteins is a more complex folding structure. The cytoskeletal protein Filamin consists of six tandem Ig repeats. The force elongation curves of this molecule exhibit the well known periodic sawtooth pattern due to the unfolding of the Ig domains. However consistently one domain (domain 4) shows an additional unfolding peak during the extension which can be explained by the existence of an "unfolding intermediate". By experiments with mutants we reconstructed the unfolding pathway of domain 4, where strand a and b break away during the first unfolding step while the rest of domain 4 (strand c,d,e,f and g) form the stable portion of the intermediate state. Moreover stretch and relaxation experiments showed additionally, that refolding from the intermediate to the native state is possible, indicating that the intermediate state forms indeed a stable structure.

Experiments on DNA in Electric Fields

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The behavior of DNA in electric fields is of great importance for many practical applications like, e.g., gel electrophoresis. We here give an overview of the fundamental electrokinetic effects involved and also of the main applications of electric field-assisted manipulation of DNA. We also present some of our experiments on DNA stretching, in particular our attempts to unfold condensed DNA in an electric field.

Quantum dots coupled to polarized leads - NRG study

Michael Sindel et al.
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Below the Kondo temperature T_K electron transport through a quantum dot (QD) containing an odd number of interacting electrons shows anomalies. A Kondo resonance (KR) in the local density of states, due to the screening of the dot spin by the lead electrons generated by an exchange coupling, is established. For this mechanism both spin species (UP and DOWN) are needed. The question what happens to the Kondo effect in QD's coupled to ferromagnetic leads, i.e. leads containing an imbalance between UP and DOWN-spins, is nontrivial since two types of correlation effects have to be considered. The Kondo resonance will obviously disappear when the leads are completely polarized. It is however of interest what the effect of partially polarized leads on transport properties is and whether the system has a strong coupling fixed point. We focus on the parallel (P) magnetization of the leads. We are computing $T=0$ properties of a model taking a finite polarization of the leads into account and study it by the NRG method.

Transient forces in dynamic atomic force microscopy

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Dynamic atomic-force microscopy (AFM) is a standard tool for the investigation of surface properties with nanometer resolution. In the tapping-mode (TM-AFM) the tip-sample interaction forces may vary substantially depending on the oscillatory state of the system. In the so-called 'low amplitude' or 'dominant attractive state' highly resolved imaging of delicate samples was demonstrated, whereas doing so in the 'high amplitude' or 'dominant repulsive state' can lead to the destruction of the sample. Thus, controlling the tip sample forces is a major prerequisite for high-resolution TM-AFM imaging in biological applications. The driving frequency as the key parameter to determine the interaction forces in TM-AFM in ambient conditions. The behaviour of tapping mode AFM is investigated with numerical simulations using the single-mode approximation as well as a multiple degree of freedom model (MDOF). With the multiple-degree-of-freedom (MDOF) approach the generation of higher harmonics and the generation of subharmonics is analyzed. Under typical imaging conditions higher harmonics are generated whereas a closer approach to the specimen surface can lead to period doubling.

The current phase relation in proximity coupled Josephson junctions

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The supercurrent between two weakly coupled superconductors is driven by the phase difference between the macroscopic wave function of the two superconductors. Thus, the current-phase relation is the fundamental characteristic of the junction. Up to now very few direct measurements of this fundamental quantity exist, in particular not for proximity coupled Josephson junctions, where the weak link is formed by a short piece of normal metal.

We present direct measurements of the current-phase relation of superconductor/normal metal/superconductor (SNS) and superconductor/dilute ferromagnet/superconductor (SfS) by means of micro-Hall magnetometry. Superconducting loops made of Al or Nb interrupted by Au wires and diluted Pd/Ni films, respectively, are fabricated by shadow evaporation.

Both types of junctions show a triangular current-phase relation at low temperatures. For longer (400 nm) Au wires, the higher harmonics of the supercurrent are gradually suppressed as the temperature is increased towards T_c . In shorter wires the current phase relation retains a triangular shape up to the much higher temperatures.

The thickness of the weakly magnetic Pd/Ni junction is chosen such that the junction is tuned into a " π "-state. For this state, the existence of a spontaneous supercurrent at zero magnetic field is predicted. An experimental signature of the spontaneous current are asymmetries in the zero field cooled hysteretic switching fields, where the magnetic flux in the loops jumps by one flux quantum. In addition the spontaneous current is directly observed in zero magnetic field as the temperature is lowered below T_c . These features are reproduced in a simultaneously deposited conventional Josephson junction when applying half of a magnetic flux quantum, whereas the magnetic response of the π -junction vanishes at this field. This directly demonstrates the existence of the longstanding prediction of the exchange field-induced intrinsic " π "-shift in the current phase relation in Josephson junctions with magnetic weak links.

Controlled release of immobilized DNA into electrolyte solution

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We report experimental data on the release of immobilized, single-stranded DNA oligonucleotides from gold electrodes into buffered electrolyte solution by an applied negative electrical bias. The temporal evolution of the desorption process is monitored by fluorescence measurements of the dye-labelled DNA and can be understood in a simple rate model.

We find that the efficiency of the desorption is predominantly controlled by the effective charge of the polyelectrolyte DNA molecule. This net (screened) charge appears to be independent over a wide range of electrolyte salt concentration in agreement to Manning's counterion condensation theory. Only above a critical ionic strength of about 0.1 M the desorption efficiency sharply decreases which we assign to a regime of excessive counterion condensation.

Engineering quantum (de)coherence in superconducting devices

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Superconducting circuits of mesoscopic size are a promising candidate for the realization of scalable quantum computers. A crucial obstacle to overcome is the decoherence from the coupling to the numerous degrees of freedom of the solid state environment and the outside world. I am going to introduce examples of such devices and review the experimental status. I will show how to engineer the decoherence properties in different ways, motivated by results of statistical physics and / or quantum information theory:

The spectrum of the environment can be shaped by filtering out the relevant frequencies, which leads to a spin boson model with a structured bath.

If more than one bath is present, such in the case of a double quantum dot charge qubit, decoherence is related to an electron flow through the device.

The impact of given, slow noise from defects in the material, can be reduced by using a dynamical decoupling scheme ("Quantum bang-bang").

By encoding quantum information in specific subspaces of the full physical Hilbert space, the quality of quantum logic gates can be improved.

I will show that the requirements of engineering decoherence differ between operation and measurement of a qubit and propose a model that implements detector-dominated measurements with long relaxation times using a spin Boson model with a peaked spectral density.

Probe lithography and chemical modification of nanometer-sized structures

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Current surface patterning techniques seem to be nearing their lowest resolution limits. Research into new techniques capable of patterning substrates is concentrated around electron beam lithography and scanning probe-based techniques as dip-pen lithography and scanning probe oxidation. The latter one has two main advantages. First it is capable of producing well-defined nanopatterned substrates with relative ease on a number of different substrates. Secondly it also introduces local groups with chemical reactivity that allows for subsequent local substrate reactions and modifications. Because a broad variety of modification reactions and compounds are available, structures created in this fashion can be employed not only in semi-conductor applications but also in sensor and smart coating devices. In this contribution the technique of local probe oxidation and subsequent chemical modification and fabrication of nanometer-sized structures on octadecyltrichlorosilane (OTS) passivated silicon wafers is presented. By applying a bias voltage on a conductive AFM-tip the OTS layer on the surface can be oxidized very locally. The oxidation changes the local properties of the surface, thus opening routes to controlled surface modification via both absorption as well as chemical modification routes. Presented here are results of the (sequential) functionalization of surfaces with (cationic) gold nanoparticles, silica particles, quaternary ammonium salts and the covalent attachment of functional silanes with for example polymerizable end-groups. Subsequently, these "functional" structures were exposed to polymerization reactions or thiol bearing proteins creating complex functional nanometer-sized structures. Also the possibility for using an automated AFM-setup for the modification of large areas will be addressed.

Poster Abstracts
1st Poster Session
28. September 2003

Low temperature single molecule spectroscopy using vibronic excitation and dispersed fluorescence detection

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We demonstrate vibronic excitation combined with spectrally resolved zero phonon line detection of single TDI molecules in both the Shpol'skii matrix hexadecane and the polymer PMMA at cryogenic temperatures. Spectral jumps as large as 80 cm^{-1} are recorded with a 1 sec time resolution. In contrast to the established zero-phonon-line excitation technique, vibronic excitation does not require a weak electron-phonon coupling, and promises applications in spectroscopy of a wide-range of single nanostructures in amorphous hosts including fluorescing proteins. This technique also enables us to determine vibrational spectra of the excited state of single TDI molecules.

Single molecule microscopy in nanostructured molecular sieves

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Center for NanoScience CeNS

Single molecule spectroscopy (SMS) is used to characterize nanometre sized structures and diffusion in the bulk volume of molecular sieves (host-guest materials). Two complementary techniques are employed: First, a single fluorophore can be analysed with a high spatial resolution with confocal microscopy. Second, a whole area of a sample can be monitored with a high temporal resolution using widefield imaging. Here we present recent investigations on two different host-guest systems.

Diffusion measurements on individual terylene diimide (TDI) molecules incorporated into various mesoporous M41S hosts have been carried out. The increased time resolution of the imaging technique makes it possible to resolve structured trajectories. These trajectories help to understand better the channel structure of the hosts and the influence of the pores on the diffusional behaviour of the guest molecules.

The second system consists of three differently sized dye molecules (Oxazine 1, 170, 750) located in $\text{AlPO}_4\text{-5}$ (AFI) crystals. Polarization dependent measurements reveal the orientational distribution of the dyes with respect to the channel structure. In addition, molecular modelling calculations on the AFI-structure are done to complement the experimental work.

Connection of Proteins to solid surfaces

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Center for NanoScience CeNS

To investigate the properties of proteins, it is important to immobilize them on solid surfaces. Until now it was necessary to develop for different proteins different methods to immobilize them. The Group of Kai Johnsson in Lausanne developed a general method for immobilization of proteins. We are trying to exploit this idea to bind Titin-GFP-Proteins covalently and specific to different solid surfaces. Once we have succeeded in doing that we can investigate the Titin-GFP with AFM.

Nanocrystals in biological applications

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We intend to use semiconductor-nanocrystals in biological applications. For example biomolecules can be labeled with these crystals and then tracked on their pathway through cells. Semiconductor-nanocrystals promise to improve this tracking compared to standard organic fluorophores as they do not bleach as fast as organic fluorescent dyes.

We use silanized and polymer coated CdSe/ZnS nanocrystals. We observed up-taking of those conjugates by different cell-types.
Another application is a motility assay for cells, build of a layer of nanocrystals.

Colloidal molecular sieves: Model system for kinetic study of crystal growth process

Boriana Mihailova
Ludwig Maximilians Universität München
Center for NanoScience CeNS

sorry, abstract not available

X-ray diffraction from ultrathin organic layers

Bert Nickel
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Center for NanoScience CeNS

Pentacene (C₂₂H₁₄), a long, flat organic molecule, is in the focus of much current research activities due to its versatile electronic properties which allow for its application in electronic devices ("plastic electronics"). The transport properties in single crystals depend strongly on the crystallographic direction since the molecules pack in a way which favors electronic transport only perpendicular to the long axis of the molecules. In turn, there is a huge interest to control the growth mode of thin films, i.e. to grow standing or lying down phases of high perfection. We have evaporated ultrathin films (1-10 monolayers) of Pentacene on oxide and metal surfaces for a broad range of deposition temperatures (200K-500K). Using X-ray scattering techniques, we observe a standing phase for deposition on SiO₂, but a lying down phase for the deposition on Ag(111). For both systems, the molecular arrangement shows a distinct dependence on the deposition temperature and film thickness. The microscopic mechanisms which control the various structures observed will be sketched.

Density Functional Simulations of Highly Reactive Mixtures

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A hypergolic mixture consists of two compounds that react spontaneously when brought into contact with one another. A mixture of monomethyl hydrazine (MMH) and nitrogen tetroxide (NTO) is an example for such a highly reactive system. It is used as a bipropellant in the upper stage engine of the European launch vehicle Ariane 5.

The ultrafast nitrogen chemistry occurring as soon as the two reactants are brought into contact with one another, is difficult to analyse experimentally. However, the short timescale and the small size of the molecules render the system suited for on-the-fly molecular dynamics, using density functional theory (Car-Parrinello molecular dynamics).

In the CPMD simulations we observe a stepwise oxidation of MMH by NTO. After each redox step a proton transfer takes place. After a few picoseconds the mixture has reacted mainly to methyl diazen and nitrous acid.

Experimental Determination of Colloidal Effective Charges

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Colloidal properties are often well described using a meanfield approach. For charged particles surrounded by an electric double layer of counter-ions a screened Coulomb potential applies. In this an effective or renormalized charge Z^* is used, which may be calculated theoretically or taken from experiments as free fit parameter with all other relevant parameters (like particle concentration or salt concentration) known. Z^* is accessible from a number of different experiments. In the present study we compare the results from conductivity, electrophoresis and elasticity measurements. We report systematic differences and correlations between charges from these experiments which need to be further understood to provide a solid base and quantitative prediction of colloid properties from charge characterisation experiments.

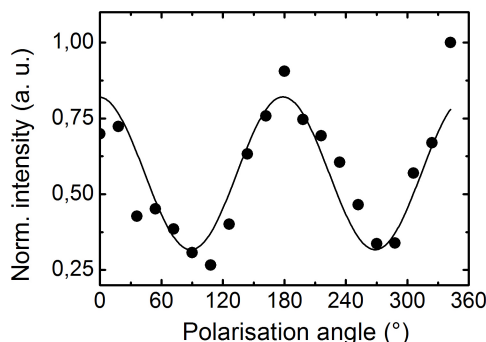
Polarised emission from single core/shell nanorods

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During the past few years considerable progress has been made in the colloidal synthesis of nanoparticles. Recently it has become possible to synthesise spherical CdSe nanocrystals with an elongated CdS shell. Here it is shown that the optical properties of the core are strongly influenced by the elongated shell. A far-field microscope is used to examine the absorption and the fluorescence of individual nanoparticles. Blinking and spectral jumps of single nanoparticles are clearly observed. Spectral jumps are assigned to the local electric field variations experienced by the nanoparticle, which arise due to the generation and annihilation of surface charges. The emission is strongly polarised, even at high temperatures. In addition, a strong polarisation anisotropy in absorption is also shown. Both clearly indicate the strong influence of an elongated shell on the absorption and emission of a spherical core.



Polarisation dependence of the emission of a single core/shell CdSe/CdS nanoparticle at 200K (black dots). The solid line shows a \cos^2 fit.

Hydrodynamics with a free surface

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A projection method for the simulation of droplets, consisting of a viscous and incompressible fluid is presented. In this kind of simulations one is confronted with the problem that the Navier-Stokes-equation has to be solved (integrated in time) in a domain that is time-dependent itself.

The three relevant physical quantities are the velocity $v(x,t)$, the pressure $p(x,t)$ and the surface, given by a level-set of a function $s(x,t)$. At all times these three variables have to fulfil the boundary conditions at the free surface. This relates the geometrical properties like tangent, normal directions and curvature to the stress-tensor of the fluid. The velocity has, due to the incompressibility, also to be divergence-free.

The presented method allows to decompose an arbitrary vector-field into parts that correspond to the physical velocity and pressure. This extends the well-known projection-method by Chorin to problems with time-dependent domains and free surfaces. A projection step like this not only gives the chance of decoupling the equations for pressure and velocity, which is the usual benefit of Chorin's method, but also yields some insight on how the time evolution of the droplet is governed by its surface.

Absorption spectroscopy on single self-assembled quantum dots

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The investigated self-assembled quantum dots are islands fabricated of semiconductor material and embedded in a different semiconductor with a larger band gap. This leads to a trapping of electrons and holes in the dots. The dots have a lateral size of a few 10nm and height of ~5nm. Due to such small dimensions the energy states of the electrons and holes in the quantum dot are quantized similar to those of electrons in an atom.

We developed a technique for measuring the absorption of light on a single quantum dot. The spectral resolution is ~100 times better than the standard photoluminescence spectroscopy which allowed already the investigation of various effects such as Zeemann-splitting and Stark-shift on single quantum dots.

With the absorption spectroscopy the fine-structure of an electron-hole pair (exciton) was measured as well as the lifetime and the oscillator strength of differently charged excitons at 4.2 K.

This was made possible by applying a gate voltage for tuning the quantum dot's energy levels and a home made confocal microscope which enabled us to measure on just one single quantum dot for several months.

Organic distributed-feedback-laser with metallic nanoparticles

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A severe obstacle to constructing organic diode lasers is the optical loss arising from metallic contacts, which generally outweighs the optical gain. We demonstrate a novel technique for contacting organic materials in laser diode structures by combining the contact and the resonator in one, using a nanostructured array of gold nanoparticles [1]. Optically pumped lasing is demonstrated in a device consisting of a conjugated polymer on top of a 2D distributed feedback template comprising gold nanodiscs on indium tin oxide. Although the nanodiscs are potential dissipative energy absorbers we find only a marginal reduction in lasing threshold when compared to conventional dielectric distributed feedback resonators. Our structures also allow an accurate control over the active lasing modes, and provide the possibility of generating two non-degenerate modes of orthogonal polarization.

[1] *A low threshold polymer laser based on metallic nanoparticle gratings*
J. Stehr, F. Schindler, J. Crewett, R. Sperling, G. von Plessen, U. Lemmer, J. M. Lupton, T. A. Klar, J. Feldmann, A. W. Holleitner, M. Forster, and U. Scherf, **Adv. Mater.** (in press)

Optimizing the Gate Performance of Coupled Solid-State Qubits

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Solid-state quantum bits are a promising candidate for the realization of a *scalable* quantum computer. However, they are usually strongly limited by decoherence due to the many extra degrees of freedom of a solid-state system. We investigate a system of two solid-state qubits in a setup that is typical for *pseudospin* solid-state quantum bits such as charge or flux systems. We evaluate decoherence properties and gate quality factors in the presence of a common and two uncorrelated baths coupling to σ_z , respectively. We show that at low temperatures, uncorrelated baths do degrade the gate quality more severely. In particular, we show that in the case of a common bath, optimum gate performance of a CPHASE gate can be reached at very low temperatures, because our type of coupling commutes with the coupling to the decoherence, which emphasizes the importance of symmetries to minimize decoherence. Moreover, we investigate Decoherence Free Subspace (DFS)-encoding schemes for capacitively coupled flux qubits to suppress decoherence during quantum gate operations with several capacitively coupled flux qubits.

For superconducting flux qubits it appears to be relatively easy to implement a tunable coupling between the qubits, if one uses tunable Josephson junctions. We evaluate possible coupling strengths and show how much extra decoherence is induced by the subgap conductance of a tunable junction. In the light of these results, we evaluate several options of using intrinsically shunted junctions and show that based on state-of-the art numbers, Josephson field effect transistors and high- T_c junctions as σ_z -shifters would be a good option, whereas the use of magnetic junctions as σ_z -shifters severely limits quantum coherence.

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Micro- and Nanofluidic on piezoelectric substrates

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Surface wave induced acoustic streaming in smallest liquid volumes is demonstrated to be a powerful tool to realize a programmable "lab-on-a-chip". Surface acoustic waves (SAW), especially Rayleigh modes, being generated on a piezoelectric substrate are shown to strongly interact with small liquid droplets and to be able to actuate the droplet along predefined trajectories. At lower SAW power, an internal streaming within the fluid leads to pronounced stirring and mixing effects. On piezoelectrics, a SAW is accompanied by strong electric fields. Those fields, propagating at the speed of sound, can also be exploited to manipulate charged or polarizable particles within a small fluid volume. We demonstrate this electro-mechanical interaction by a SAW induced orientation and alignment of carbon nanotubes.

A second prominent mode of SAW on piezoelectrics are shear waves. Those modes of elastic energy lack of a vibration component normal to the substrate surface which makes them ideally suited for sensor applications in a liquid. We give several examples for such applications, including the detection of electrolyte conductivity.

In situ hybridization of DNA oligonucleotides detected by gold conjugated nanoparticles and Atomic Force Microscopy

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A common antigen detection system in biological studies is based on antibodies conjugated to fluorescent labels. The spatial resolution and sensitivity of this system is strictly linked to the resolution of optical microscopy and the stability of the fluorescent label. With gold conjugated antibodies, sensitive high resolution immuno-cytochemistry for the detection and quantification of proteins and nucleic acids is also possible in electron microscopy (EM). Since EM need dried samples to be investigated, the sample preparation procedures can affect the native structure of biological samples.

The aim of this study was to localize specific DNA oligonucleotides after *in situ* PCR or hybridization by gold conjugated nanoparticles. The DNA probes were labelled with digoxigenin and the detection system was based on antibodies against digoxigenin conjugated with gold particles. In some cases the immuno gold labelling was amplified by a colloidal silver enhancement. To detect hybridized DNA we used atomic force microscopy (AFM) that generates topographic and three-dimensional images on a nanometer scale in ambient and liquid conditions without destroying the sample morphology. The experimental setup was demonstrated on specific probes against human leukaemia, epidermal growth factor receptor after *in situ* PCR on human metaphase chromosomes and specific oligonucleotides on stretched plasmid DNA.

We present results on amplified gold particles on human chromosomes after *in situ* PCR and *in situ* hybridization, suggesting potential applications for high-resolution physical mapping of human genes and disease correlated genes.

AlPO₄-18 synthesized from colloidal precursors and its use for the preparation of thin films

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The interest in the preparation of microporous materials in the form of colloidal suspensions containing nanocrystals with narrow particle size distribution is driven by their numerous useful applications. The most interesting aluminosilicate zeolites from an industrial point of view have been prepared in the form of stable colloidal suspensions containing nanocrystals with a narrow particle size distribution. However, amongst the aluminophosphate based microporous materials, only the AFI-type material was synthesized in colloidal form.

Here we report the preparation of nanosized AlPO₄-18 (AEI-type topology) with a monomodal particle size distribution from colloidal precursor solutions. Further the AlPO₄-18 nanocrystals were employed for the preparation of ultra-thin films on silicon wafers *via* spin coating and additional crystal growth at elevated temperature. Dynamic light scattering and conventional X-ray diffraction were used to follow the crystal growth of AlPO₄-18 in colloidal solutions. The mean radius of the final AlPO₄-18 crystals was about 80 nm, and according to the X-ray analysis they were completely crystalline after 48 h hydrothermal treatment. The structural evolution of the thin films was studied with grazing incidence diffraction using synchrotron X-ray radiation. The diffractograms of spin coated and grown AlPO₄-18 films at various incident and exit angles were recorded and they reflect the crystal orientation along the film thickness as a function of the preparation conditions.

Poster Abstracts
2nd Poster Session
29. September 2003

New energy/electron donor-acceptor triads based on *bis*-terpyridine ruthenium(II) complexes and perylene

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Understanding energy/electron transfer processes between organic/organic as well as organic/inorganic entities, also on a molecular level, has become of increasing interest over the last few years.^{1,2} We report here on the synthesis and characterization of a new class of triad molecules which include one perylene acceptor and two *bis*terpyridyl Ru(II) complexes. Concerning the synthetic strategy, first an easily accessible terpyridine functionalized perylene was synthesized by reaction of amino-pentyl-terpyridine³ with perylene-tetracarboxylic-acid-dianhydride (PTCDA). Subsequently the well-known Ru(III)/Ru(II) coupling method together with unfunctionalized terpyridine was applied in order to yield the donor-acceptor-donor triad. Attempts to increase the bad solubility in common solvents were performed as well by using poly(ethylene glycol)-functionalized terpyridine as "endcapping" complex ligand. Characterization included NMR spectroscopy, MALDI-TOF mass spectrometry, UV/Vis spectroscopy as well as cyclic voltammetry. First PLE measurements revealed that only the complexed triad, in contrast to the uncomplexed respectively the Ru(III)-mono-complexed species, showed an energy/electron process occurring from the Ru(II) complex to the perylenebisimide core. Further time-resolved measurements, also including better soluble systems, will reveal the true nature of this process.

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DNA-based nanocircuits

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Due to its unique molecular recognition properties DNA is one of the most promising molecules for the rational assembly of nanoscale electronic circuits. In order to achieve this goal, several key problems have to be solved: In order to connect DNA-based structures to the outside world, DNA has to be positioned reproducibly and accurately within conventional nanostructures like, e.g., metal electrodes. As DNA itself is not conductive, it has to be chemically modified to render it useful for nanoscale electronics. Finally, in order to build complex circuits from DNA, non-trivial self-assembly schemes have to be developed. We here report on our efforts to solve these problems.

Lab on a chip: Nanostructured building units for parallel analysis

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sorry, abstract not available

Coiled Coil Unzipping

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As recent experiments have shown is the Coiled Coil structure a truly elastic one. This means that at forces about 25 pN the Coiled Coil starts unfolding and is able to refold against an external force.

But the exact distribution of the stabilisation Forces between the two strands is still unknown. Therefore we plan to "unzip" the Structure with means we use a Titin(repeat 1-4) Coiled Coil Dimer Structure and try to dissociate both strands by using the AFM.

Combining near field microscopy and infrared spectroscopy

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In our lab at the Max-Planck-Institut für Biochemie, we operate a scattering-type (apertureless) scanning nearfield infrared microscope (s-SNIM)¹. By using the (locally) confined near field of scattered light at an AFM-tip one can overcome the Abbe-limit and get a spatial resolution of some ten nanometers even at wavelengths of ten microns.

As we want to measure both amplitude and phase of the backscattered light, a coherent light source has to be used for illuminating the tip. For this reason, we currently use mainly gas lasers (CO₂ and CO). Laser light is very monochromatic and we therefore only get information about the optical properties of the sample at the selected wavelength. Getting spectroscopic information involves taking images sequentially at various laser lines.

To overcome this time-consuming procedure, we plan to use a new source of broadband but still coherent light. One such source are pulsed lasers. We plan to use Ti:Sapphire lasers, convert the frequency from the visible region to the infrared by nonlinear crystals, and then bring this light to our tip.

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Electronic transport through molecular systems

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We present a numerical method for the calculation of electronic transport through molecular systems. It uses methods taken from quantum chemistry combined with a scattering matrix approach to calculate a bias dependent transmission function. The current is then obtained by use of the Landauer formula. We also present results for a calculation of phenylene-diisocyanide SAMs (self assembled monolayers) attached to gold leads and compare them to experimental data.

The Physics of Polyplexes

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Nanometer scale structures have garnered significant interest due to their potential use in a variety of applications ranging from biomaterials for pharmaceuticals to the microelectronics industry.

Especially of late, a heavy emphasis has been placed on systems that can self-assemble on the nanometer scale with the ability to control both the size and complexity of the system. We focus on the complexation behavior in polyelectrolyte melts comprised of calf-thymus DNA complexed with various polycations. Small-angle x-ray scattering (SAXS) experiments were used to determine the internal structure in these "polyplexes" and their dependence on various external parameters.

Hexagonal packing of the DNA was observed for all systems with a variation in both the internal spacings and the degree of internal order which was highly dependent on the specific polycation used. An electrostatically induced phase transition was observed with increasing salt concentration. This first order phase transition and complex dissolution again showed dependence on the polycation and scale approximately with the respective binding energies of the polyplex. Compressibility was also investigated, as a function of salt, in these systems by osmotic stress measurements.

Molecular Force Sensors

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AFM-Experiments on modular proteins containing the Green Fluorescent Protein reveal that one can mechanically unfold this medium-sized protein. It unfolds at pulling forces around 75 pN and shows a short-lived (~100 µsec) unfolding intermediate state.

Since the fluorescence of the protein vanishes once unfolded, our experiments suggest that the GFP could act as a in-vitro and in-vivo molecular force (-threshold) sensor.

In the future we hope to correlate fluorescence behaviour of single GFP's with AFM force curves by a combined setup.

Encapsulation of molecular nanowires in porous hosts

Barbara Fieres

sorry, abstract not available

Investigation of single polyelectrolyte molecules adsorbed on solid supports by the use of an AFM

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AFM based force spectroscopy is a powerful method that allows the measurement of intra- and intermolecular forces of single molecules. It also allows the investigation of polyelectrolyte desorption from solid supports which was recently shown for polyvinylamine.

We extended our work to the investigation of further polymers like polyacrylic acid or DNA.

Polyelectrolytes normally show weak interactions with the surface with high exchange rates. Therefore our measurements take place in thermal equilibrium and we observe desorption plateaus in the force spectra instead of rupture forces. For the electrostatic contribution we expect a linear dependency on the salt concentration in solution. We were able to show this linear dependency of the desorption force on the concentration of NaCl ions in solution for surfaces with fixed surface potential. Apart from the electrostatic contribution also non-coulombic interactions between the polymers and the surfaces like hydrophobic or coordinative contributions were characterized. Additionally intermolecular interactions between two or more polyelectrolyte molecules could be observed if divalent metal ions were present in solution.

In conclusion we can say that single molecule force spectroscopy provides a lot of information that helps to understand the mechanisms of polymer adsorption on solid surfaces that build the basis for a variety of applications.

Dynamics of Excitons in Coupled Quantum Well Structures

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The experiments to learn more about motion and interaction of long-living excitons in coupled quantum wells (QW) [1, 2] are carried out in semiconductor heterostructures at low temperatures (4 K). These epitaxially grown samples contain two GaAs-QWs, which are separated by a thin $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ tunnelling barrier. Using photo and electron beam lithography nano-patterned gate A photo-generated exciton can be polarized by means of an electrical field orientated perpendicularly to the QW layer. This means the electron and its associated hole are located in different QWs. The energy level of this so-called spatially *indirect exciton* is lower compared to a direct exciton (electron and hole in the same QW). This energy shift is due to the Quantum Confined Stark Effect (QCSE) in coupled QWs. In addition, the overlap of the electron and hole wave function is reduced by the thin tunnelling barrier resulting in a lower probability of recombination, i.e. the excitonic life time increases significantly. This is experimentally observed using a time and energy resolved pump-and-probe setup to investigate the emitted photoluminescence.

According to the geometry of the gates applied to the samples the excitonic energy can be modulated laterally. Due to this voltage tuneable gradient field the long-living indirect excitons drift in-plane [3, 4]. An experimental setup using an intensified CCD-Camera with a temporal resolution in the sub-nanosecond regime allows detailed studies on the dynamics of the excitonic drift. An optimized geometry of the gate structures will be developed with regard to form voltage controlled *excitonic traps*.

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Use of an organic template structure for the manipulation of nano-scale objects

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The adsorption of Trimesic Acid (TMA) to various single crystal surfaces has been studied under Ultra High Vacuum and ambient conditions. The self-assembled structure is characterized by periodic non-dense-packing of the molecules. Depending on the preparation method, two different network structures could be realized. In both cases, induced by directed hydrogen bonding, the organic molecules built a two-dimensional grid architecture with molecular caves - both able to store guest molecules at specified adsorption sites.

As a first step TMA molecules (Fig. 3) themselves were inserted as guest molecules into the host structure. The guest molecules could be identified in two different vertical and 6 different horizontal adsorption sites. In the horizontal case STM induced switching of a single guest molecule to six stable positions was observed. The states of this molecular switch have a distance of 0.15 nm. The calculated energy barriers indicating that the switch is stable at room temperature are consistent with the experiment.

Furthermore Bucky-Balls (Fig. 2) could be inserted in the hollow sites. With a diameter of about 0.7nm C_{60} fits easily in the pores of the TMA structure which have a diameter of about 1.5 nm. By means of STM the Bucky-Balls could be imaged within the template structure and be directly kicked from one cell to another.

As a third example coronene molecules (Fig. 3) were co-crystallized after the host structure was formed. With a diameter of about 1nm coronene molecules also fit quite well into the open pores. Closed layers of TMA with every cavity filled by a coronene molecule could be imaged. Even the submolecular structure of coronene can be seen in the STM images. By applying voltage pulses the guests molecules could controllably be kicked out of the cavities.

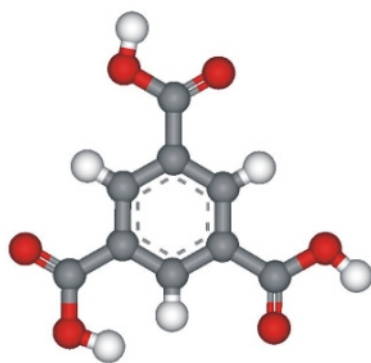


Fig. 1 Trimesic Acid - $C_9H_6O_6$

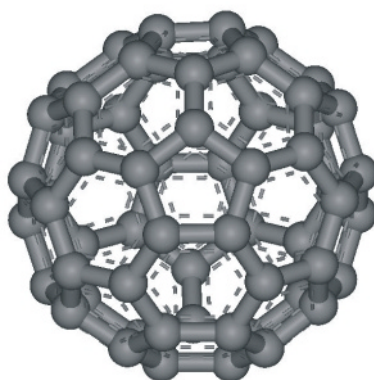


Fig. 2 Buckminsterfullerene - C_{60}

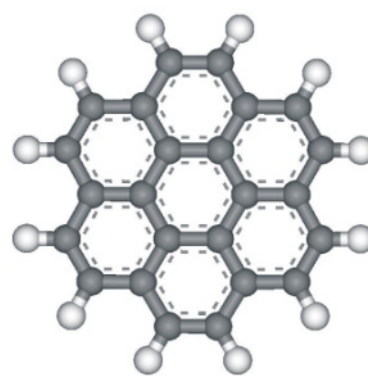


Fig. 3 Coronene - $C_{24}H_{12}$

Quantum Chemical Simulation of Photoreactions in Nanosystems

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A classical example of a photoreaction in a nanosystem is the unidirectional cis-trans isomerisation of the chromophore in rhodopsin. The retinal protonated Schiff base isomerizes from the 11-cis to the all-trans form, initiating the process of vision. We have simulated the process using restricted open-shell Kohn-Sham (ROKS) theory [1, 2] in combination with a QM/MM approach [3].

At high temperatures we find that the C11-C12 double bond rotates to 90 degrees in the excited state. Remarkably, this change of the dihedral angle is accompanied by very small atom displacements only.

Similar photochemistry is found in the light-driven unidirectional nanorotor by Feringa [4]. With ROKS simulations we are able to elucidate the mechanism that leads to unidirectional motion. The cis-trans isomerization can occur only in one direction with minor atom displacements.

Rotation in the other direction would afford large-scale movements of the bulky rests. Such a motion is nearly impossible if the dynamics of the system is taken into account.

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Compensation of telegraph noise decoherence by means of bang-bang control

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With growing success in isolating solid-state qubits from external noise sources the origins of decoherence inherent of the material start to play a relevant role. One representative example are charged impurities in the disordered substrate or junction material, which produce typical telegraph noise and can hence be modeled as bistable fluctuators (b.fl.) [1,2]. In order to demonstrate the possibility of the active suppression of the disturbance from a *single* fluctuator, we theoretically implement an elementary bang-bang control protocol [3,4]. We simulate numerically the random walk of the qubit state on the Bloch sphere with and without bang-bang compensation scheme and compare it with analytical results we receive by use of appropriate Langevin equations in the long-time limit. Hereby we find out, that the deviation of the pure b.fl. random walk is scaled down approximatively by the ratio of the bang-bang period and the typical flipping time of the fluctuator. Therefore we expect the bang-bang control working as a high pass filter on the spectrum of noise sources. This indicates, how the influence of $1/f$ -noise ubiquitous to the solid state world could be reduced. We also derive two generic and analytically solvable random walk models to describe non perfect bang-bang pulses and evaluate their extra dissipating influence on the qubit. So we build a realistic picture, how effective our idealized bang-bang scheme might be in practice and which the technical limitations are for using this concept in fighting decoherence generated by material defects.

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Decoherence and Cotunneling of Charge States in Double Quantum Dots

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Quantum computation requires a sufficient quantum coherent time evolution. Therefore it is of central importance to minimize decoherence through external baths in particular in solid state systems. We study a quantum dot charge qubit, where basis states are defined by the position of an additional electron in the system of two coupled quantum dots [1], i.e. one can find this electron either on the left or the right dot. The coupling of these two states can electrostatically be controlled by a tunneling barrier between the two dots.

We provide a theoretical analysis of the decoherence (due to cotunneling processes to the leads and due to the coupling to phononic modes) of this system by using the Bloch-Redfield theory. This theory is well established in chemical physics and treats internal couplings of a system exactly and couplings to external baths perturbatively.

An analysis of the cotunneling transport through this system reveals a rich, non-monotonic behaviour of the stationary current depending on the internal degrees of freedom [2].

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Cell chamber for the AFM measurement of cells

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Measuring the mechanical properties of cells can give insight into the processes in the living cell as well as they can give informations about the influence of chemicals or pharmaceuticals on the cell and on its physiological processes. For long-time measurements of the mechanical properties of living cells, physiological and sterile ambient conditions have to be provided to the cell culture during the measurement. Therefore we set up a cell chamber around our AFM, including a temperature and CO₂ control. Additionally together with IBIDI a liquid cell chamber has been adjusted for the AFM, that provides a microfluidic channel for the fast exchange of the culture medium and the easy addition of small amounts of chemicals. First experiments with different types of cells show, that the cells can be measured for several hours. In the following steps, the elasticity of the cell membrane shall be observed under the influence of different exogenous agents with statical and dynamical methods.

Structure of Large Molecules forming Self-Ordered Monolayers - a Scanning Tunneling Microscopy (STM) Study and Theoretical Simulation

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Large molecules forming well-ordered monolayers find possible applications in coatings, catalysts, photo-active materials, molecular electronics, and more. Because it is still hard to predict, which (large) molecules have self-ordering properties, investigations of supramolecular architectures (self-ordered assemblies) are important for the basic understanding of both intermolecular and molecule-substrate interactions. We deposited dendritic compounds via solution-casting at ambient conditions on HOPG. Domains, stacking faults, superstructures and seldom single defects can be observed in the self-ordered monolayers. The general ordering strategy is based on alkyl chain interaction and π -stacking. By synthesizing and investigating new dendritic molecules, we additionally found the central part of these molecules to be of some importance in the ordering process. An averaging analysis on a large statistics of molecules lead to high-resolution images displaying sub-molecular resolution on individual molecules. A theoretical simulation provides additional information for the understanding of the molecular ordering on the HOPG-surface.

Surfaces as Molecular Workbenches

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Two types of surfaces are used as molecular workbenches for the manipulation of single biomolecules.

First, cationic lipid layers prepared on hydrophobic or hydrophilic surfaces force DNA molecules to adsorb onto the lipid plane. On fluid lipid layers the DNA is horizontally mobile allowing the use of fluorescence microscopy to study the dynamic behavior of single DNA molecules.

Therefore, the DNA molecules serve as model 2D-polymers and their behavior has been compared to different polymer theories. Moreover, this system offers broader possibilities. For a molecular workbench it is desirable to relocate, position, stretch, separate, and analyze single DNA molecules. The first goal, relocation, can be achieved with electric fields. The movement of single DNA molecules under the influence of electric fields has been studied previously. Currently, nanostructured surfaces are used to force long DNA threads (50 000 bps) to orient along one direction and form a straight linear molecule. A theory has been developed to explain this phenomenon. In the future, the straightened conformation of the DNA will allow for the study of the dynamic interaction with single proteins by fluorescence microscopy. This molecular workbench could be adapted to serve for other charged biomolecules as well.

Second, T5 phages have been found to attach to a hydrophobic plastic surface. A constant flow is applied and the protein FhuA which triggers the ejection of the phage DNA is added. The ejection process can now be monitored in vitro with fluorescence microscopy. The ejection process takes place within less than 1 sec. DNA always stays attached to the phage. It seems that there are three different sizes of ejected DNA molecules: 8, 15, 24 μm .

Imaging of self-assembled organic adsorbates

STM-measurements under UHV and ambient conditions

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The adsorption of trimesic acid (TMA) on single crystal surfaces has been studied under Ultra High Vacuum and ambient conditions. In ambient conditions the TMA-molecules were measured at the liquid-solid interface, while in UHV trimesic acid was evaporated on different substrates using an effusion cell.

The resulting topology is one of periodic, non-dense-packed TMA molecules, induced by directed hydrogen bonding. Two coexisting phases have been imaged by STM with sub-molecular resolution in our group. The organic molecules form a two-dimensional grid architecture with molecular caves in both cases.

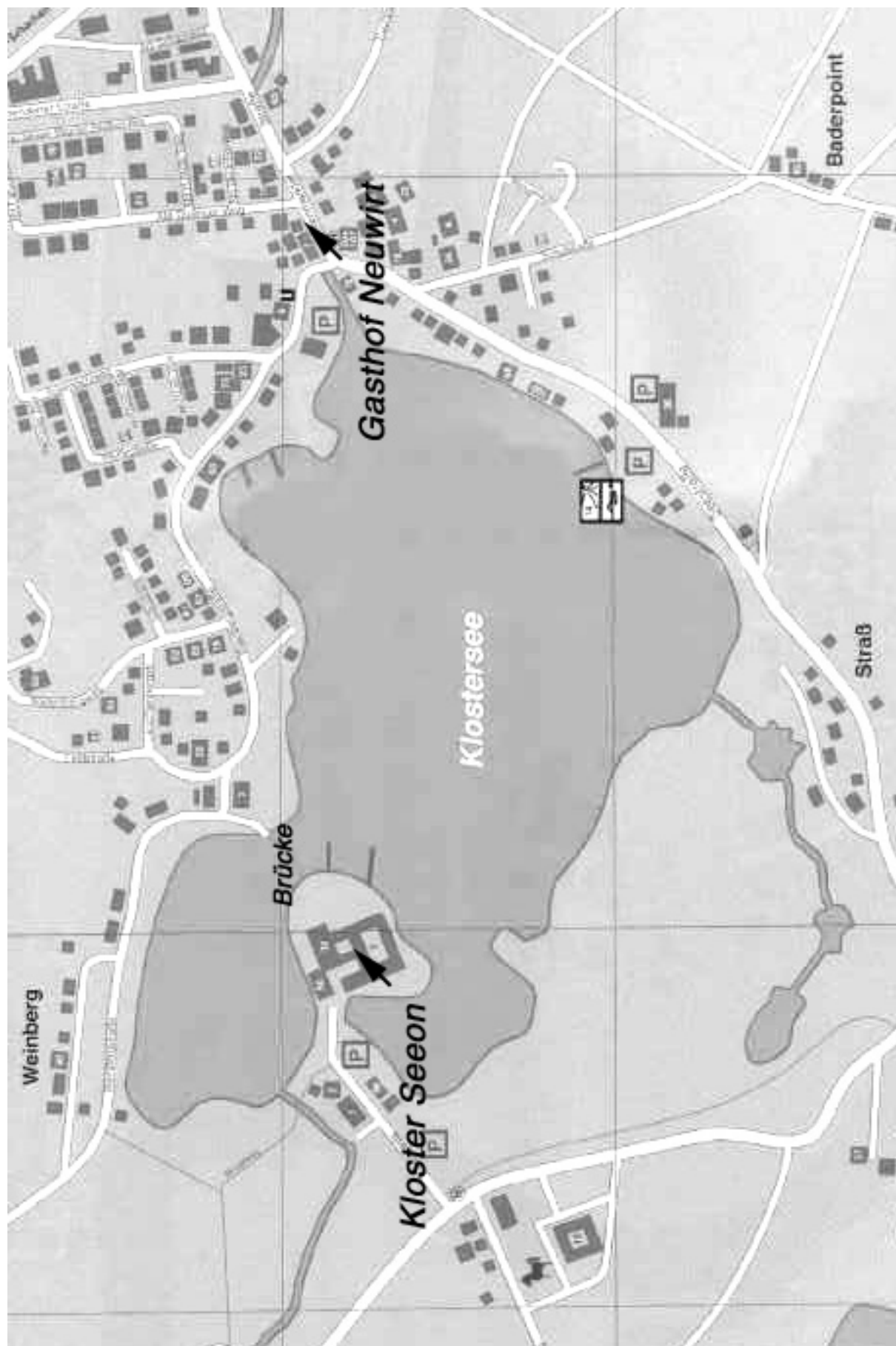
For the resulting grid network the preparation method is crucial. Therefore further examination of the preparation specifics is in progress.

This grid network is now being used as host in a host-guest-architecture. A diverse number of molecules can be introduced as guests into this architecture for a wide variety of expected uses ranging from ligand stabilized gold clusters ($\text{Au}_{55}(\text{PPh}_3)_{12}\text{Cl}_6$) as a base for growth of protein crystals to suggested technological uses like data storage.

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10.00 - 24.00 Uhr
Montag - Dienstag Ruhetag
10 min vom Kloster Seeon

Kloster Seeon Express

Fahrtrichtung: Bad Endorf ? Kloster Seeon (Montag-Freitag)

Haltestelle ab	Haltestelle an
Bad Endorf Bahnhof 07.50	Kloster Seeon 08.27
Bad Endorf Bahnhof 11.50	Kloster Seeon 12.27
Bad Endorf Bahnhof 13.40	Kloster Seeon 14.17

Fahrtrichtung: Kloster Seeon ? Bad Endorf und Prien (Montag-Freitag)

Haltestelle ab	Haltestelle an
Kloster Seeon 11.10	Bad Endorf Bahnhof 11.47
Kloster Seeon 12.45	Bad Endorf Bahnhof 13.36
Kloster Seeon 16.40	Prien Bahnhof 17.22 (ICE ab 17.42)

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