CPP 30 POSTER: Chemical physics

Zeit: Dienstag 16:30–18:30 Raum: Poster TU D

CPP 30.1 Di 16:30 Poster TU D

Nucleosomal repositioning studied with single molecule FRET spectroscopy — •Alexander Gansen, Florian Hauger, Katalin Toth, and Jörg Langowski — Deutsches Krebsforschungszentrum, Abteilung: Biophysik der Makromoleküle, Im Neuenheimer Feld 580, 69120 Heidelberg

Fluorescence resonance energy transfer (FRET) has proven to be an important tool to investigate conformational and structural dynamics in vivo and in vitro. We use a confocal Single Pair - FRET system to analyse molecules diffusing freely in solution. Particles are detected by means of single photon counting and subsequent burst selection. Test experiments on doubly labelled DNA oligomers are presented that show the abilities and the limitations of the method.

Recent experiments focus on the analysis of the structure and dynamics of reconstituted mononucleosomes. SpFRET verified the bulk measured FRET efficiency of 15-20

CPP 30.2 Di 16:30 Poster TU D

Fluorescence lifetime fluctuations of single molecules in polymer films — •Ruben Schmidt and Frank Cichos — Photonik und Optische Materialien, Institut für Physik, TU Chemnitz, 09107 Chemnitz

The dynamical processes in polymers close to the glass transition involve a wide range of relaxation timescales, which leaves the glass transition in part still not well understood. We employ single fluorescent molecules to probe local fluctuations of the polymer environment to give more detailed information on the glass transition itself. We present measurements of fluorescence lifetime fluctuation of single dye molecules embedded in thin polymer films. While modifications of the radiative rate of the dye molecules due to local density fluctuations are not observed, fluctuations due to non-radiative channels based on conformational changes of the dye molecule are found. Statistical analysis of these fluctuations allow tracking of environmental fluctuations over 3 to 4 orders of magnitude in time.

CPP 30.3 Di 16:30 Poster TU D

Quantum optical applications of single molecule spectroscopy with vibronic excitation — •Wolfgang Marquardt[1], Alper Kiraz[2], Özgur Müstecaplioğlu[2], Moritz Ehrl[2], Christoph Bräuchle[1], and Andreas Zumbusch[1] — [1]Department Chemie, Ludwig-Maximilians Universität München, Butenandtstr. 11, 81377 München, Germany — [2]Department of Physics, Koç University, Rumelifeneri Yolu, 34450 Sariyer, Istanbul, Turkey

Low temperature single molecule spectroscopy often rely on excitation of the purely electronic zero-phonon-line (ZPL). Because the absorbing ZPL is so narrow, already small spectral jumps lead to a loss of the excitation. Here we report vibronic excitation combined with spectrally resolved ZPL detection as a novel technique for single molecule spectroscopy at cryogenic temperatures. In contrast to ZPL excitation, vibronic excitation benefits from broad absorption bands (broadened by 1-10 ps lifetimes and phonon sidebands) allowing the investigation of large spectral jumps [1]. We demonstrate that with our technique, also ultralong coherence times can be obtained by recording only the purely electronic zero-phonon line emission of single molecules. It will be shown that With single molecule emission of this type, quantum optical phenomena like two-photon interference can be observed [2]. Finally, our approach promises applications in spectroscopy of a wide-range of molecular systems including polymers and fluorescing proteins.

[1] A. Kiraz, M. Ehrl, C. Bräuchle, A. Zumbusch, J. Chem. Phys. 118, 10821 (2003) [2] A. Kiraz, M. Ehrl, C. Bräuchle, A. Zumbusch, Appl. Phys. Lett. 85, 920 (2004)

CPP 30.4 Di 16:30 Poster TU D

Dynamics of Photoinduced Charge Ejection of CdSe Nanocrystals in Dielectric Environments — •Abey Issac[1], F. Cichos[2], and C. von Borczyskowski[1] — [1]Optical Spectroscopy and Molecular Physics,Center for Nanostructured Materials and Analytics, Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Photonics and Optical Materials,Center for Nanostructured Materials and Analytics, Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Fluorescence intermittency (blinking) of single CdSe/ZnS quantum dots (QDs) obeys power law statistics for the lifetime of the dark states. This power law distribution is supposed to be related to a distribution of states located outside the QDs, which are able to trap charges ejected from the QDs. We present for the first time direct evidence, that blinking is affected by the polarity of the surrounding medium. The higher the dielectric constant of the medium, the higher will be the probability for long off times. To explain the observed results we propose a simple self-trapping model for the ejected charges. The interaction of the reaction field, induced by the ejected charge in the matrix, with the ejected charge stabilizes the charge against a fast return to the ionized particle. On the other hand, the lifetime statistics of the bright periods (on times) is unaffected by the dielectric environment and shows a turnover between two power laws. We relate this turnover to an intermediate step during the ionization of the QDs involving surface states.

CPP 30.5 Di 16:30 Poster TU D

A modified sfa setup for single molecule tracking — •Arne Schob and Frank Cichos — Photonics and optical materials, Institute of physics, TU Chemnitz, 09107 Chemnitz

A surface forces apparatus (sfa) is a well established technique to study liquid-substrate interactions in ultrathin confined films on mesoscopic lengthscales. Shear experiments whithin a sfa can help understanding friction with ultrathin lubricant layers more detailed allthough a conventional sfa is limited to ensemble measurements. Tracking of single molecules could be of tremendous benefit here, because anisotropies and inhomogeneities in the molecular diffusion can easily be revealed.

For the first time we present a surface forces apparatus, which has been modified to provide access to molecular motion within confined liquids using single fluorescent molecule tracking. Force-distance-curves of our setup demonstrate that a capacitive position sensor is able to replace the common interferometrical thickness measurement. With a separation of external force driven motion (shear) from stochastic driven diffusion we demonstrate the possibility to investigate molecular details of confined liquids under shear, which may serve as a model for ultrathin lubricant layers between solid surfaces.

CPP 30.6 Di 16:30 Poster TU D

Optische Pinzetten zur Untersuchung Molekularer Motoren — •Stephan Wörmke, Christoph Bräuchle und Jens Michaelis — Department für Chemie, LMU München, Butenandtstrasse 11, 81377 München

Molekulare Motoren spielen für viele Prozesse innerhalb von Zellen eine wichtige Rolle. Sie können, einer Maschine ähnlich, chemische Energie in mechanische Arbeit umsetzen. Die mechanischen Eigenschaften dieser Moleküle können auf Einzelmolekülbasis mit Hilfe von Optical Tweezers untersucht werden. Diese nutzen den Strahlungsdruck, um im Fokus eines stark fokussierten Lasers Teilchen mit hohem Brechungsindex zu fixieren.

Wir präsentieren hier den Aufbau eines Zweistrahl Optical Tweezers, mit dem es möglich ist, durch Messung von Impulsänderungen direkt die auf ein Partikel wirkende Kraft zu bestimmen. Im Falle von DNA basierten Molekularen Motoren sind zwei verschiedene Experimentiermodi möglich, wobei jeweils die DNA zwischen zwei Polystyrolkugeln befestigt wird, von denen eine in der optischen Falle gehalten und die andere an der Spitze einer Mikropipette fixiert wird. Zum einen kann die Position der auf der Mikropipette befestigten Kugel konstant gehalten und die infolge der Motoraktivität resultierende Kraft gemessen werden, um die Maximalkraft (Stallforce) eines Molekularen Motors zu bestimmen. Zum anderen kann die zwischen den zwei Kugeln wirkende Kraft konstant gehalten werden, indem die Position der Mikropipette über einen Regelkreis in Echtzeit nachführt. So können charakteristische Änderungen der Motoraktivität bestimmt und die mechanochemischen Eigenschaften abgeleitet werden.

CPP 30.7 Di 16:30 Poster TU D

High-resolution spectroscopy of exciton states in single light-harvesting complexes of purple bacteria — •Philipp Reichl, Jürgen Baier, Martin Richter, Silke Oellerich, and Jürgen Köhler — Experimental Physics IV, University of Bayreuth

The initial steps in bacterial photosynthesis involve the absorption of photons by light-harvesting complexes (LH1 and LH2) and subsequent transfer of the excitation energy to the reaction center.

The crystal structure of LH2 complexes shows that the chromophores are arranged in two concentric rings embedded in the protein scaffold. Chromophores in the inner ring are separated by less than 10 Å. This leads to strong coupling and the formation of delocalized exciton states, which show broad bands in the spectrum. If disorder breaks the symmetry of the arrangement, an additional narrow line (k=0 transition) can be observed in the spectrum. From the fluorescence lifetime a linewidth of 150 MHz is predicted for this transition.

In order to detect this transition we have expanded our experimental setup to include two lasers, the first for spectral localization in a wide spectral region, the second with a linewidth of 500 kHz for high-resolution scans of the k=0 transition.

CPP 30.8 Di 16:30 Poster TU D

Visualisation, Kinetics, and Thermodynamics of Biomolecular Interactions — •F. Schubert[1], H. Zettl[1], M. Lysetska[1], M. Drechsler[2], Y. Talmon[3], G. Krauss[4], and G. Krausch[1] — [1]Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth — [2]Makromolekulare Chemie II, Universität Bayreuth, 95440 Bayreuth — [3]Department of Chemical Engineering, Technion, Haifa 32000, Israel — [4]Laboratorium für Biochemie, Universität Bayreuth, 95440 Bayreuth

We have examined the interactions of DNA and replication protein A (RPA) with atomic force microscopy (AFM), cryo-transmission electron microscopy (cryo-TEM), surface plasmon resonance (SPR), and fluorescence correlation spectroscopy (FCS) to gain a better understanding of structure, kinetics and thermodynamics.

The AFM experiments show a length decrease of the dsDNA upon UV irradiation. Adding RPA to undamaged DNA, only a small amount of complexes with terminal binding can be found. Upon binding of RPA to UV-damaged DNA a length decrease and appearance of globular structures occur. In order to exclude the influence of the mica surface the same experiments were performed using cryo-TEM.

The analysis of SPR and FCS data of ssDNA–RPA interactions includes the determination of the rate constants, the equilibrium constant, and the Gibbs free energy. By performing the reaction at different temperatures, it is possible to extract thermodynamic information about the system. The two methods yield different values for ΔG but almost the same value for ΔH. Thus there has to be a difference in ΔS, which may be due to a different degree of freedom for the DNA.

CPP 30.9 Di 16:30 Poster TU D

Absorption spectra for a model light-harvesting system using non-Markovian theories — •M. Schröder, U. Kleinekathöfer, and M. Schreiber — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Different methods for obtaining the linear absorption spectrum of a simplified model of the B850 ring of the photo-synthetic system of purple bacteria are compared. Starting from a quantum master equation, the frequency domain spectrum can be obtained within linear response theory. In these quantum master equations one often decouples the population dynamics from that of the coherences (secular approximation) and neglects memory effects (Markov approximation). The absorption spectra of the ring aggregate resulting from the Redfield theory with and without secular approximation are compared to those results from a time-local and a time-nonlocal non-Markovian theory [1]. This is done without [2] and with averaging over the static disorder. Though the difference between the different levels of approximation is small after the disorder averaging, it is clearly visible for single samples.

[1] U. Kleinekathöfer, J. Chem. Phys. **121**, 2505–2514 (2004).
[2] U. Kleinekathöfer, M. Schröder and M. Schreiber, J. Lumin. (in press)

CPP 30.10 Di 16:30 Poster TU D

Ultraschnelle photoinduzierte Prozesse in biologisch relevanten Chromophorsystemen — •Benjamin Dietzek[1], Raman Maksimenka[1], Gudrun Hermann[2], Wolfgang Kiefer[1], Jürgen Popp[3] und Michael Schmitt[3] — [1]Institut für Physikalische Chemie, Universität Würzburg — [2]Institut für Biophysik und Biochemie, Universität Jena — [3]Institut für Physikalische Chemie, Universität Jena

Licht-induzierte Prozesse in biologisch relevanten Systemen zeichnen sich durch die hohe Effizienz des biologisch vorteilhaften Prozesses gegenüber dissipativen Konkurrenzprozessen aus. Für das Verständnis von Prozessen in biologischen Systemen ist es somit notwendig, die Voraussetzungen für diese hohe Selektivität zu charakterisieren. Für die Charakterisierung solcher biologisch relevanten Systeme wie zum Beispiel der Protochlorophyllid-Oxidoreduktase ist eine Beschreibung der unmittelbar auf die Lichtabsorption folgenden ultraschnell ablaufenden strahlungslosen Deaktivierungsprozessen notwendig. Die ultraschnell ablaufenden Prozesse im Protochlorophyllid A Chromophor wurden als Basis für zeitaufgelöste Messungen an dem Chromophor-Enzym-Komplex charakterisiert. Die Beschreibung dieser Primärprozesse wurde mittels fs-zeitaufgelöster transienter Absorption und der transienten Gitter-Spektroskopie mit einer Zeitauflösung von 80 fs vorgenommen. Diesen Ergebnissen werden Messungen an dem strukturell ähnlichen Magnesiumoctaethylporphyrin zum Vergleich gegenübergestellt.

CPP 30.11 Di 16:30 Poster TU D

Investigation of field dependent CIDNP in multinuclear radical pairs: Determination of magnetic interaction parameters in tryptophan radicals by comparison with model calculations — •Karsten Miesel[1], Konstantin Ivanov[2], Alexandra Yurkovskaya[2], and Hans-Martin Vieth[1] — [1]Department of Physics, Free University of Berlin, D-14195 Berlin, Germany — [2]International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

The magnetic field dependence of chemically induced dynamic nuclear polarisation (^{1}H-CIDNP) formed in reversible electron transfer reaction between triplet excited dyes (2,2'-dipyridyl and anthraquinone-2-sufonate) and N-acetyl-tryptophan in aqueous solutions at varying pH was observed and compared to model calculations. The experiment employs fast field cycling between a variable field of polarization ranging from 0 to 7T and the fixed field of a cryomagnet for high resolution NMR detection. At high field the CIDNP depends on both g-factors and hyperfine interactions (HFI) of the radicals, while at low field it is conditioned solely by HFI. The difference between magnetic resonance parameters for cationic and neutral radicals of tryptophan is discussed. The entanglement of spins in the tryptophan radicals formed at zero magnetic field was unravelled by Fourier-analysing the dependence of the CIDNP spectral pattern on the duration of the NMR rf excitation pulse. This approach provides information about the populations of all involved nuclear spin states and allows verifying the HFI constants obtained from simulations of the CIDNP field dependence.

CPP 30.12 Di 16:30 Poster TU D

Short-lived radicals of purine bases in aqueous solution: reactivity and characterization by magnetic resonance — •Alexey Kiryutin[1,2], Olga Morozova[2], Alexandra Yurkovskaya[2], and Hans-Martin Vieth[1] — [1]Department of Physics, Free University of Berlin, D-14195 Berlin, Germany — [2]International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

The structure of nucleic acids and the mobility of their bases can be probed by the effects of dynamic nuclear spin polarization (CIDNP) created in reversible photoreactions between individual bases and suitable organic dye molecules. For quantitative studies detailed information on the reactions of the dye with the basic building blocks is required. The quenching of triplet excited 2,2'-dipyridyl by the two purine nucleotides guanosine and adenosine monophosphate (GMP and AMP) and the subsequent radical pair decay is a prototype of such a reaction. Laser flash photolysis and CIDNP techniques were applied to get information on the quenching rates and the mechanism of this chemical process and on the structure of the radicals so formed as a function of the pH of aqueous solution. By time-resolved CIDNP the influence of the secondary process of degenerate electron exchange between AMP and its cation radical was studied. For GMP and AMP the CIDNP was measured at variable magnetic field (0..7 T). From simulation of these field dependencies the hyperfine couplings and g-factors of the short-lived neutral, anionic and cationic forms of the nucleoside radicals were determined.

CPP 30.13 Di 16:30 Poster TU D

Structure and Magnetic Resonance Parameters of the Cation-Radicals of Methionine as Studied by the CIDNP Magnetic Field Dependence — •Sergey Korchak[1,2], Konstantin Ivanov[2], Alexandra Yurkovskaya[2], and Hans-Martin Vieth[1] — [1]Department of Physics, Free University of Berlin, D-14195 Berlin, Germany — [2]International Tomography Center of SB RAS, 630090, Institutskaya 3a, Novosibirsk, Russia

Radical intermediates as they play a key role in many photoreactions often elude spectroscopic characterization because of their high reactivity resulting in a lifetime too short for direct observation. An indirect method exploiting the dynamic spin polarization created in the paramagnetic reaction stage and conserved in the diamagnetic reaction product

circumvents this problem. Such a Chemically Induced Dynamic Nuclear Polarization (CIDNP) formed in the reactions of methionine (Met) and N-acetylmethionine (NMet) with triplet excited 4-carboxybenzophenone (CBP) was measured in an external magnetic field of 0-7 Tesla in neutral and basic aqueous solution. The results show that at a pH above 9, the Met cation radical exists in a cyclic form with a two-center three-electron bond between the nitrogen and sulfur atoms, whilst at pH below 9 the Met cation radical has a linear structure. Cation radicals of NMet are formed in linear structure only. By comparing the experimental results with model calculations the g-factors and the hyperfine constants of the cyclic and linear cation radicals were determined. Experimental method and simulation technique will be discussed.

CPP 30.14 Di 16:30 Poster TU D

Theoretical investigation of the reactivity of Mg deposited on PTCDA films — •L. Mancera, R. Scholz, A. Abbasi, M. Schreiber, B.A. Paez, G. Gavrila, G. Salvan, and D.R.T. Zahn — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

In this work, the spectroscopic changes observed upon deposition of Mg on PTCDA films of 15 nm thickness are investigated with different microscopic models for Mg-PTCDA compounds. The Raman spectra obtained on these films reveal pronounced changes of the vibrational fingerprint, indicating the reactive nature of the PTCDA/Mg interface. Some of the new modes observed after Mg deposition can be assigned to modified molecules with magnesium atoms attached to the oxygen atoms in the carboxylic and anhydride groups. In a geometry resembling crystalline PTCDA, the energetically most favourable position for a single Mg atom was found in a bridge position between the oxygen end groups of two adjacent PTCDA molecules. The shift of the $2p$ core levels of the Mg atoms observed in photoemission spectroscopy results from a significant positive net charge on the Mg atoms, in keeping with the Mulliken charge and core level shift found in the calculation. Due to the delocalized nature of the lowest unoccupied states of neutral PTCDA, the additional negative charge is distributed over the entire molecular area, resulting in relatively small shifts of the O_{1s} and C_{1s} core levels.

CPP 30.15 Di 16:30 Poster TU D

Surface properties and haptic perception of soft surfaces — •Denys Zimin[1], Kristin Schmidt[1], Meik Ranft[2], Margit Harsch[3], Jan Sandler[3], Volker Altstädt[3], and Georg Krausch[1] — [1]Physikalische Chemie II, Universität Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany — [2]BASF AG, 67056 Ludwigshafen, Germany — [3]Polymere Werkstoffe, Universität Bayreuth, Universitätsstrasse 30, 95447 Bayreuth, Germany

We study the physical properties of various polymer and leather surfaces (roughness, hydrophobicity, deformability, elasticity and morphology), aiming towards an objective measure of haptic perception of these surfaces by test persons. The surfaces are characterized by subjective evaluations (smooth/rough, waxy, sticky, pleasant/unpleasant, dry, etc). Correlations between the subjective evaluations and the physical properties are discussed.

CPP 30.16 Di 16:30 Poster TU D

SFM as a Model System for Local Impact — •Alexander Gigler[1], Sabine Hild[1], Stefan Walheim[2], Othmar Marti[1], and Thomas Schimmel[2] — [1]Experimental Physics, University of Ulm, D-89069 Ulm — [2]Institute for Nanotechnology, Forschungszentrum-Karlsruhe GmbH, D-76021 Karlsruhe

For surface characterization using Scanning Force Microscopy (SFM) the understanding of tip-sample interactions is a crucial point. Normal and lateral forces act during such experiments and have to be investigated at the same time to find out the correlations between them. To model these forces a method called Dynamic Friction Force Microscopy (DFFM) has been added to an existing Digital Pulsed Force Mode (DPFM). The crash of a head of a hard-disk into the disk is an example for such an impact. Since this event happens at high speeds (meters per second), the setup has been extended to this range of relative tip-sample velocity.

CPP 30.17 Di 16:30 Poster TU D

Organically doped sol-gel materials for applications in photodynamic therapy and optical sensing — •Halina Podbielska[1,2], Agnieszka Ulatowska-Jarza[1,3], Uwe Bindig[3], HansJ. Eichler[2,3], and Gerhard Müller[4] — [1]Bio-Optics Group, Institute of Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, PL-50370 Wroclaw, Poland — [2]Institute of Optics, Technical University Berlin, Strasse des 17 Juni 135, D-10623 Berlin, Germany — [3]Laser-und Medizin-Technologie Berlin, Fabeckstr. 60-62, D-14195 Berlin, Germany — [4]Charite Universitätsmedizin Berlin, Campus Benjamin Franklin, Institut für Medizinische Physik und Lasermedizin, Fabeckstr. 60-62, D-14195 Berlin, Germany

The optical properties of photosensitive dyes as may be used for photodynamic therapy or for sensing, entrapped in silica sol-gels, are examined. Our idea is to construct a fiberoptic light applicator which can act as a carrier for photosensitizers. Two photoagents were examined: protoporphyrine PP IX and chlorophyll based Photolon, immobilized in sol-gel coatings on optical fibers. Absorption and emmission spectra were measured in air and varous environments. It was shown that the dyes preserve their chemical activity, do not leave sol-gel pores, and may contact with even large molecules from external environment. Additionaly, we observed that photosensitizers entrapped in sol-gel coatings are sesnitive to hydrogen ions, so thus they can be used for pH sensing.

CPP 30.18 Di 16:30 Poster TU D

Holographische Untersuchungen an azobenzolhaltigen Blockcopolymeren — •Michael Häckel[1], Lothar Kador[1], Carsten Frenz[2] und Hans-Werner Schmidt[2] — [1]Physikalisches Institut und BIMF, Universität Bayreuth, 95440 Bayreuth — [2]Makromolekulare Chemie I und BIMF, Universität Bayreuth, 95440 Bayreuth

Verschiedene Diblock-Copolymere, die in ihren Seitenketten Azobenzol-Chromophore und zum Teil zusätzlich mesogene Gruppen enthalten, wurden auf ihre Eignung als Medium für volumenholographische Datenspeicher untersucht. Die in einem holographischen Gitter auf Grund der Chromophorreorientierung erreichbare Brechungsindexmodulation sowie die Stabilität der eingeschriebenen Gitter wurden in Abhängigkeit verschiedener Parameter gemessen. In Proben mit einer Dicke von 1 mm wurde das Verhalten beim Einschreiben mehrerer Gitter unter verschiedenen Winkeln ("Winkel-Multiplexing") untersucht. An der selben Stelle der Probe konnten bis zu 200 Gitter eingeschrieben und eindeutig ausgelesen werden.

CPP 30.19 Di 16:30 Poster TU D

Photo- and thermo-induced aging of azobenzene layers — •Burkhard Stiller, Norman Mechau, Marina Saphiannikova, and Dieter Neher — University of Potsdam, Institute of Physics-Soft Matter Physics- Soft Matter Physics, Am Neuen Palais 10, 14469 Potsdam

We have studied the process of photo- and thermo-induced aging of thin azobenzene layers spin coated from tetrahydrofurane solution onto a glass substrate. The first cycle, when the film was either illuminated by visual light or annealed above the glass transition temperature, Tg, causes an abnormal hardening which manifests itself as an increase of elastic modulus of the layer. Additionally, diffusion of small dye molecules within the layer can be observed below Tg in the first heating cycle. In all subsequent cycles the layer shows a normal softening, whereas no diffusion below Tg can be observed. We ascribe the abnormal hardening in the first cycle to abrupt relaxation of excess free volume left in the layer by rapid solvent evaporation during spin coating process.

CPP 30.20 Di 16:30 Poster TU D

Combined IR and VIS ellipsometric study of polymer films — •Karsten Hinrichs[1], Michael Gensch[1], Norbert Esser[1], Karin Sahre[2], Jürgen Pionteck[2], and Klaus-Jochen Eichhorn[2] — [1]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [2]Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden, Germany

Ellipsometry in the mid infrared (MIR) [1] and Visible (VIS) spectral range have been cooperatively applied for the measurement of optical constants of various polymer films: e.g polyimides, poly(n-butyl methacrylate) and poly(vinyl chloride) layers on gold and silicon substrates. Such optical constants are important e.g. for studies with mixed systems or as input parameters for other methods, such as scanning near field microscopy or attenuated total reflection spectroscopy. Simulation and interpretation of the ellipsometric spectra in optical layer models

allowed the determination of the thickness, the high frequency refractive index and the parameters of molecular vibrations of the different polymer compounds. The optical constants of the single compounds served as input data for the analysis of miscibility, composition and structure in thin films [2,3]. [1] K. Hinrichs, D. Tsankov, E.H Korte, A. Röseler, K. Sahre, K.-J. Eichhorn, Appl. Spectrosc. 56 (2002) 737. [2] G. Dlubek, G. Pompe, J. Pionteck, A. Janke, D. Kilburn, Macromol. Chem. Phys. 204 (2003) 1234. [3] N.A. Nikonenko, K. Hinrichs, E.H. Korte, J. Pionteck, K.-J. Eichhorn, Macromolecules 37 (2004) 8661.

CPP 30.21 Di 16:30 Poster TU D

Spectroscopy and Photoswitching of Single Photochromic Nanostructures — •Stephan Rath, Mark Heilig, and Helmut Port — 3. Phys. Inst. Uni Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart

There is increasing interest in possible application of photochromes in thin film technology. By using UHV-vapor deposition methods, specific thin film variants can be fabricated reproducibly: (a) amorphous dots and (b) nano-crystals of adjustable size and distance, respectively, but also (c) extended films with homogeneous coverage. All forms are stable at room temperature. Because of their optical bistability, derivates of fulgides and diarylethenes have been chosen. Films on different substrates have been prepared, optical properties and photochromic performance in the film variants are differentiated. For single nanostructures their fluorescence spectra have been studied with respect to size dependence and structural constraints. On samples with structure distances below the optical diffraction limit, addressing and photo-switching of individual nanostructures between the two isomeric forms is performed by scanning near-field optical microscopy (SNOM).

CPP 30.22 Di 16:30 Poster TU D

Ultrafast Excited-State Excitation Dynamics in a quasi-1D Light-Harvesting-Antenna based on Ru(II) and Pd(II) Chromophores — •Benjamin Dietzek[1], Wolfgang Kiefer[1], Jörg Blumhoff[2], Lars Böttcher[2], Sven Rau[2], Dirk Walther[2], Jürgen Popp[3], and Michael Schmitt[3] — [1]Institut für Physikalische Chemie, Universität Würzburg — [2]Institut für Anorganische Chemie, Universität Jena — [3]Institut für Physikalische Chemie, Universität Jena

A detailed study on the excited state excitation hopping taking place within a multicenter complex is presented. The charge transfer is initiated by the photoexcitation into the lowest metal-to-ligand charge-transfer band of one of the peripheral Ru(II) chromophores and terminates on the central Pd(II)-subunits. Thus, the system under investigation can be thought of as a model system for an extremely simple quasi-1D inorganic-light-harvesting antenna. The kinetic steps involved in the overall process are inferred from femtosecond time-resolved transient-grating kinetics recorded at spectral positions within the spectral regions of ground state bleach and transient absorption. The data leads to the formulation of a model for the intra-molecular excitation hopping that ascribes intersystem crossing and subsequent cooling to the two fastest among the recorded processes. Following these initial steps charge transfer from the Ru- to the one of the Pd-chromophores is observed. A 220 ps-component that is observed in the ground state recovery only is attributed to excitation hopping between the two identical Pd-chromophores.

CPP 30.23 Di 16:30 Poster TU D

Effect of the substitution in azulene derivatives investigated by means of fs transient grating and transient absorption spectroscopy. — •Raman Maksimenka[1], Benjamin Dietzek[1], Torsten Siebert[1], Adriana Szeghalmi[1], Dirk Rausch[2], Christoph Lambert[2], Wolfgang Kiefer[1], and Michael Schmitt[3] — [1]Institut für Physikalische Chemie, Universität Würzburg — [2]Institut für Organische Chemie, Universität Würzburg — [3]Institut für Physikalische Chemie, Universität Jena

Azulene and its derivatives have been thoroughly investigated, due to their unusual photophysical behaviour, such as dipolar character, long wavelength absorption and the violation of Kasha's rule. Owing to these features, azulene has been incorporated into a number of organic materials, e.g. molecular switches and chromophores with nonlinear optical properties. Here we demonstrate the effect of chemical substitution on the excited state dynamics of three azulene derivatives, in which azulene acts as a π-bridge substituted by an acceptor and a donor. In comparison with the weak azulene absorption band, each of these azulene derivatives shows an unusually intense CT band at around 400-500 nm. Decay channels of the electronic states of these azulene derivatives are explored by means of fs transient grating and transient absorption spectroscopy. In all experiments non-monoexponential decays indicate a complex structure of the excited states. In conclusion, fs transient grating and transient absorption spectroscopy were applied to the investigation of the effect of substitution in azulene derivatives on the structure and the dynamics of the excited states.

CPP 30.24 Di 16:30 Poster TU D

Transient EPR Study of Electron Transfer in Photosystem I: A0 to A1(Anthraquinone) to FX — •Irina Karyagina[1], Yulia Pushkar[2], and Dietmar Stehlik[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Calvin Laboratory, Physical Biosciences Division, Lawrence Berkeley National Laboratory, Berkeley, California, 94720-5230

In Photosystem I (PS I) phylloquinone (PhQ) acts as a low potential electron acceptor during light induced electron transfer (ET). The origin of the very low midpoint potential is investigated by introducing the lower potential acceptor anthraquinone (AQ) into the A1 site of PS I in the presence and absence of the partial negative charge on the iron-sulphur clusters (FeS). Using multi-frequency transient EPR spectroscopy, structural and dynamic properties of the sequential radical pair (RP) states are investigated. The orientation of AQ in all samples is the same as that of PhQ in native PS I. The kinetics show: (i) ET from the second to the third RP is faster from AQ than from PhQ to FeS as expected from the more negative reduction midpoint potential of AQ. (ii) By the same change of midpoint potential the preceding ET step from the first to the second RP is slowed down. The lifetime of the first RP state is observed to lengthen with increasing temperature. This unusual temperature dependence and the observed changes in spin polarisation pattern are explained by a model based on a distribution of lifetimes/midpoint redox potentials of A0.

CPP 30.25 Di 16:30 Poster TU D

X-ray Absorption Spectromicroscopy of the Copper-Oxygen Complex in the Respiratory Protein Haemocyanine — •A. Krasyuk[1], A. Oelsner[1], G. Schönhense[1], M. Möller[2], H. Decker[2], M. Pohl[3], U. Kleineberg[3], and U. Heinzman[3] — [1]Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz — [2]Institut für Biophysik, Johannes Gutenberg - Universität, 55099 Mainz — [3]Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld

We report on XANES investigations at the copper $L_{2,3}$ edges and oxygen K-edge of haemocyanine molecules in aqueous TRIS buffer solution (or dehydrated) using photoemission electron microscope. The experiment [1] has been performed at the undulator beamline UE56/1 SGM at BESSY II. Although the investigated molecules (24-mere with a volume of 20 x 20 x 10nm^3) contain only 48 Cu atoms, the Cu $L_{2,3}$ absorption edges at 930 eV (L_3) and 948 eV (L_2) are clearly detectable. A spectromicroscopic analysis of different regions of a micrometer-size haemocyanine cluster reveals two different Cu species with the position of the L_3 signal showing a chemical shift of about 1 eV. This is the size of shift expected for the difference between monovalent Cu (as present in the deoxy-state) and the divalent Cu (present in the oxy-state), as measured for copper oxides [2]. Measurements in the O K XANES region above 530 eV photon energy reveal strong differences in the oxygen XANES, again showing similarities with the corresponding spectra for Cu oxides. Financial support by BMBF (05 KS1 UMC-0) and DFG (SFB 625, project B5) is gratefully acknowledged. [1]M. Pohl et al., Ultramicroscopy (2004) in print, [2]M. Hävecker, Dissertation TU Berlin (2000).

CPP 30.26 Di 16:30 Poster TU D

X-ray Absorption Spectromicroscopy of the Copper-Oxygen Complex in the Respiratory Protein Haemocyanine — •A. Krasyuk[1], A. Oelsner[1], G. Schönhense[1], M. Möller[2], H. Decker[2], M. Pohl[3], U. Kleineberg[3], and U. Heinzman[3] — [1]Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz — [2]Institut für Biophysik, Johannes Gutenberg - Universität, 55099 Mainz — [3]Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld

We report on XANES investigations at the copper $L_{2,3}$ edges and oxygen K-edge of haemocyanine molecules in aqueous TRIS buffer solution (or dehydrated) using photoemission electron microscope. The experiment [1] has been performed at the undulator beamline UE56/1 SGM at BESSY II. Although the investigated molecules (24-mere with a volume of 20 x 20 x 10nm^3) contain only 48 Cu atoms, the Cu $L_{2,3}$ absorption edges at 930 eV (L_3) and 948 eV (L_2) are clearly detectable. A spectromicroscopic analysis of different regions of a micrometer-size haemocyanine

cluster reveals two different Cu species with the position of the L_3 signal showing a chemical shift of about 1 eV. This is the size of shift expected for the difference between monovalent Cu (as present in the deoxy-state) and the divalent Cu (present in the oxy-state), as measured for copper oxides [2]. Measurements in the O K XANES region above 530 eV photon energy reveal strong differences in the oxygen XANES, again showing similarities with the corresponding spectra for Cu oxides. Financial support by BMBF (05 KS1 UMC-0) and DFG (SFB 625, project B5) is gratefully acknowledged. [1]M. Pohl et al., Ultramicroscopy (2004) in print, [2]M. Hävecker, Dissertation TU Berlin (2000).

CPP 30.27 Di 16:30 Poster TU D

Phase behavior of confined asymmetric binary liquid mixtures: Theoretical analysis of experimental data — •Dirk Woywod, Gernot Rother, Sebastian Schemmel, Gerhard H. Findenegg, and Martin Schoen — Stranski-Laboratorium, TU Berlin, Sekr. TC 7,Straße des 17. Juni 124, 10623 Berlin

We investigate the phase behavior of an asymmetric binary liquid mixture between two planar homogenous substrates (slit pore). We employ a lattice-gas model and a mean-field approximation to obtain a closed expression for the grand potential.

This model is applied to study the phase behavior and microscopic structure of a iso-butyric acid (iBA) + heavy water (D_2O) liquid mixture confined to mesoporous silica matrices (CPG-10). Confinement-independent model parameters are adjusted to match the experimental coexistence curve in the bulk. Since the pore liquid is in equilibrium with an external reservoir we can also fix the thermodynamic state in the model. By choosing appropriate values of the pore width and the attraction strength between substrates and water we analyze the impact of confinement on the phase diagram. Apart from a depression of the liquid+liquid critical point we observe surface-induced phase transitions as well as water adsorption by the walls [1]. The theoretical predictions are supported by differential refractometry data and small-angle neutron scattering measurements.

[1] D. Woywod, S. Schemmel, G.H. Findenegg, and M. Schoen, J. Chem. Phys., (sub. 2004)

CPP 30.28 Di 16:30 Poster TU D

Elastische Streuung von Synchrotronstrahlung an freien Nanopartikeln — J. Shu[1], K. R. Wilson[1], M. Ahmed[1], S. R. Leone[1], •C. Graf[2] und E. Rühl[2] — [1]Department of Chemistry and Lawrence Berkeley National Laboratory, University of California, Berkeley, California, 94720, U.S.A. — [2]Institut f. Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Es werden erste Resultate zur winkelaufgelösten, elastischen Lichtstreuung im Bereich $82 \leq \lambda \leq 155$ nm an freien, sphärischen Silica-Nanopartikeln mit Durchmessern zwischen 100 nm und 240 nm vorgestellt. Die Partikel werden aus wässriger Lösung in die Gasphase überführt und im Vakuum zu einem Strahl fokussiert. Es bilden sich dabei isolierte Nanopartikel und Aggregate. Es zeigt sich eine intensive Vorwärtsstreuung der Vakuum-UV-Strahlung sowie erste Hinweise auf Mie-Moden. Mie-Simulationen zeigen für die isolierten Partikel eine gute Übereinstimmung mit den experimentellen Daten. Abweichung werden dagegen für Proben beobachtet, die Aggregate enthalten. Die Resultate belegen, dass mit diesem neuen Ansatz freie Nanopartikel charakterisieren lassen. Ebenso können Informationen zur Breite der Größenverteilung der Nanopartikel abgeleitet werden.

CPP 30.29 Di 16:30 Poster TU D

Density functional study of the phase behavior of bidisperse ferrocolloids in external fields — •Gabriel M. Range and Sabine H. L. Klapp — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Sekretariat TC 7, Fakultät II für Mathematik und Naturwissenschaften, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin, Germany

The phase behavior of bidisperse ferrocolloids, consisting of binary mixtures of dipolar hard spheres (DHS), is investigated using density functional theory in the modified mean-field approximation. We focus on the fluid phase regime, where we consider both isotropic and anisotropic phases.

In the absence of external magnetic fields our results reveal complex fluid-fluid phase behavior involving demixing and first- and second-order isotropic-to-ferroelectric phase transitions. Dependent on the asymmetry of the mixture, measured by a parameter Γ, we encounter three different types of phase behavior, differing in the degree to which demixing dominates the system.

In strong magnetic fields we observe only two such types distinguished by the behavior of the line of triple points. External fields have negligible effect on the demixing transitions of weakly asymmetric mixtures, while gas-liquid transitions are influenced similarly to the one-component case. Strongly asymmetric mixtures, however, show a strong destabilization of the high-temperature coexistences which are the result of an interplay of demixing and ordering transitions.

CPP 30.30 Di 16:30 Poster TU D

Counterion condensation and effective charge of polyelectrolytes — •Ulrich Scheler and Ute Böhme — Leibniz Institute for Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden

Electrostatic and hydrophobic interactions dominate the interaction of proteins with other molecules and surfaces. Electrophoresis NMR is applied to investigate the effective charge of polyeletrolytes, proteins and complexes. The charge is derived from the hydrodynamic friction determined in the diffusion experiment and the electrophoretic mobility free of any model. In water only 10-20

CPP 30.31 Di 16:30 Poster TU D

Colloidal 3D Photonic Crystals with Au55-Clustermaterials — •Birgit Mellis[1], Günter Schön[1], Günter Schmid[2], and Ulrich Simon[3] — [1]Institut für Anorganische Chemie/ Festkörperchemie, Universität Duisburg-Essen, Schützenbahn 70, 45127 Essen — [2]Institut für Anorganische Chemie, Universität Duisburg-Essen, Universitätsstr.5-7, 45117 Essen — [3]Institut für Anorganische Chemie und Elektrochemie, RWTH Aachen, Prof.-Pirlet-Str.1, 52074 Aachen

A new kind of 3D-Photonic Crystal (PhC) showing bandgaps in the UV-Vis region is presented here. It is designed by the chemical bottom-up method out of suspensions of monodisperse polystyrene particles coated completely by monolayers of watersoluble Au55-nanoclusters. The crystals are prepared by different assembling strategies and the resulting bandgaps characterized by UV-Vis spectroscopy. The degree of order in the crystals is controlled by Atomic Force Microscopy and Optical Microscopy. Through choosing the polystyrene particle size the gap position of the PhCs can be tailored. The Au55-nanoclusters as ligandstabilized quantum dots show Single Electron Tunneling (SET) at room temperature through the ligand barrier between two adjacent clusters. The combination of photonic bandgap behaviour with SET in one system can serve as a means of lossless intern energy or information transfer between photons and electrons, a problem which has not been solved yet for PhCs.

CPP 30.32 Di 16:30 Poster TU D

Photophysics of Dynamic Phenomenon at the Quantum Dot Surface — •Mohamed Abdel-Mottaleb[1], Thomas Blaudeck[2], Frank Cichos[2], and Christian von Borczyskowski[1] — [1]a Optical Spectroscopy and Molecular Physics, Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany — [2]Photonics and Optical Materials, Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

Understanding of the optical properties of quantum dots is of growing importance due to the potential applications of such systems. Of main importance is the quantum dots intermittence. Generally, a proposed explanation for this phenomenon is the charge transfer from the quantum dot to the surrounding medium. The surrounding medium is though of as a distribution of traps that can either reside on the nanoparticle surface itself or in a close proximity to it. In either situation, the surface of the nanoparticle will play an important role in this phenomenon. Thus, the understanding, and eventually the control, of quantum dot intermittence is dependent on both the nature of the traps and that of the quantum dot surface.

Using a combination of steady-state titration and time resolved florescence we will demonstrate the dynamic nature of the quantum dot surface and propose a simple procedure to influence the dynamic processes occurring at the surface. Furthermore, through the introduction of organic molecules to the surface, we studied the organic-quantum dot interactions.

CPP 30.33 Di 16:30 Poster TU D

A TEM and XANES study of vanadium oxide nanotubes — •A. Gloskovskii[1], S. A. Nepijko[1], G. Schönhense[1], A. Reiber[2], H. A. Therese[2], G. H. Fecher[2], H. C. Kandpal[2], C. Felser[2], W. Tremel[2], and M. Klimiankou[3] — [1]Institut für Physik, Johannes Gutenberg - Universität, 55099 Mainz — [2]Institut für Anorganische und Analytische Chemie, Johannes Gutenberg - Universität, 55099 Mainz — [3]Institut für Materialforschung I, Forschungszentrum Karlsruhe GmbH, 76021 Karlsruhe

The vanadium oxide nanotubes used in this study were synthesized using the sol-gel technique following the procedure reported by Krumeich et al. [1]. TEM studies of vanadium oxide nanotubes show that the samples consist of multi-walled nanotubes with inner diameters in the range of 20-40 nm, and a length of typically several μm (it can even reach tens of μm). Spectroscopic measurements were performed to understand the electronic state of vanadium in relation to bulk material. The EDX and EELS measurements revealed that the chemical formula of the nanotubes is V_2O_5. Comparison of XAS measurements taken from nanotubes and bulk V_2O_5 revealed an overall similarity but also significant differences in details between their spectra. The latter can be explained by a major contribution of the surface to the electronic structure and electronic transitions of V_2O_5 nanotubes in comparison to bulk material. Band structures for both bulk and slab V_2O_5 were calculated by LMTO and FLAPW methods showing a good agreement with the experiment.

(This work is funded by the DFG in SFB 625 TP9.)

[1] F. Krumeich et al.; J. Am. Chem. Soc. 121, (1999) 8324

CPP 30.34 Di 16:30 Poster TU D

Stockmayer fluids under the influence of confining disordered materials — •Carsten Spöler and Sabine H.L. Klapp — Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 124, 10623 Berlin, Germany

The phase behavior of fluids is very sensitive to the nature of the intermolecular interactions as well as to the presence of a confining material on a nanometer scale. Our work bases on integral equation theory (Reference Hypernetted Chain Approximation) in combination with the replica method and we consider Stockmayer fluids (i.e. fluids containing dipolar and Lennard-Jones interactions) exposed to disordered porous matrices (e.g. silica aerogels). The model matrices consist of hard spheres, hard spheres with additional Lennard-Jones matrix-fluid interaction or dipolar hard spheres. For all confined systems a remarkable shift of the boundaries of the homogeneous isotropic high temperature phase, relative to the bulk fluid, is observed as shown on this poster.[1,2] The treatment of the orientational dependence of the dipolar potential is cumbersome but angle-averaged potentials (like the Keesom potential) are known to produce reasonable well predictions of the condensation transition for the bulk Stockmayer fluid (as long as the dipole moment remains relative small). Therefore, we also test the performance of angle-averaged potentials for our confined systems.[3] [1] C. Spöler and S.H.L. Klapp, J. Chem. Phys. 118, 3628 (2003) [2] C. Spöler and S.H.L. Klapp, J. Chem. Phys. 120, 6734 (2004) [3] C. Spöler and S.H.L. Klapp, J. Chem. Phys. 121, 9623 (2004)

CPP 30.35 Di 16:30 Poster TU D

Depletion force between two large spheres suspended in a bath of small spheres: Onset of the Derjaguin limit — •Martin Oettel — Max–Planck–Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany

We analyze the depletion interaction between two hard colloids in a hard–sphere solvent and pay special attention to the limit of large size ratio between colloids and solvent particles which is governed by the well–known Derjaguin approximation. For separations between the colloids of less than the diameter of the solvent particles (defining the depletion region), the solvent structure between the colloids can be analyzed in terms of an effective two–dimensional gas. Thereby we find that the Derjaguin limit is approached more slowly than previously thought. This analysis is in good agreement with simulation data which are available for a moderate size ratio of 10. Small discrepancies to results from density functional theory (DFT) at this size ratio become amplified for larger size ratios. Therefore we have improved upon previous DFT techniques by imposing test particle consistency which connects DFT to integral equations. However, the improved results show no convergence towards the Derjaguin limit and thus we conclude that this implementation of DFT together with previous ones which rely on test particle insertion become unreliable in predicting the force in the depletion region for size ratios larger than 10.

M. Oettel, Phys. Rev. E **69**, 041404 (2004).

CPP 30.36 Di 16:30 Poster TU D

Raman spectroscopy on metallic single-walled carbon nanotubes under electrochemical doping — •Peter Rafailov — Institut für Festkörperphysik der Technischen Universität Berlin, Sekr. PN 5-4, Hardenbergstr. 36, D-10623, Germany

We report a Raman investigation of the high-energy modes of metallic single-walled carbon nanotubes (SWNTs) upon electrochemical doping. We found these modes to be extremely sensitive to quite low doping levels which is manifested in large frequency shifts and dramatic intensity redistribution within the high-energy Raman band. These phenomena are explained by a possible removal of a Peierls-like instability that governs the softening of the high-energy modes in metallic carbon nanotubes.

CPP 30.37 Di 16:30 Poster TU D

Photophysics of Single Supramolecular Aggregates of Semiconductor Nanoparticles and Organic Molecules — •Thomas Blaudeck and Frank Cichos — Photonics and Optical Materials, Institute of Physics, TU Chemnitz, 09107 Chemnitz, Germany

We report on elementary interaction processes in aggregates of self-organized thiol-end-capped organic molecules and semiconductor nanoparticles (NPs). In the regime of strong coupling between individual NPs, delocalization of the electronic states across multiple NPs leads to new states and yields a change of optical and electronic properties by environment. In this respect, steady-state spectroscopy of CdSe NPs in solution shows significant red-shifts of the band-edge exciton in both absorption and emission spectra as the concentration of 1,4-Benzenemethanethiol (BDMT) is increased. This fact is interpreted as an indication for the aggregation process. Photoluminescence of the aggregates reveals a spectral variation correlated with size. We also present results on the single-particle scale approached by confocal microscopy, spectroscopy and time-correlated single-photon counting (TCSPC).

CPP 30.38 Di 16:30 Poster TU D

Scaling Properties of Dendrimers — •Ulrich Scheler and Bernd Fritzinger — Leibniz Institute for Polymer Research Dresden, Hohe Str. 6, D-01069 Dresden

A scaling exponent for PAMAM dendrimers with varying terminal groups in methanol is derived from the molar-mass dependence of the hydrodynamic radius. The hydrodynamic radius is calculated from the diffusion coefficient, measured by PFG NMR, using the Stokes-Einstein-equation. The dependence of the hydrodynamic radius from molar mass is compared with a simple geometrical model, a scaling law and a branching model by Kataoka. Values of the scaling exponent are 3.2 for PAMAM-NH2 and PAMAM-OH and 3.8 for PAMAM-COONa. The simple geometric model gives the best fit to the data.

CPP 30.39 Di 16:30 Poster TU D

Amphiphilic Colloidal Particles at the Water-Air and the Water-Dodecane Interface — •Reinhard Sigel[1], Lakshmanan Sannachi[1], Javier I. Amalvy[2], and Steve P. Armes[2] — [1]Max-Planck-Institut of Colloids and Interfaces, Am Mühlenberg 1, D-14476 Golm — [2]University of Sussex, Brighton, UK

For sterically stabilized polystyrene latex particles it was shown before that they reduce the surface tension of water [1]. This amphiphilic property is due to the [2-(dimethylamino)ethyl methacrylate-block-methyl methacrylate] [PDMA-b-PMMA] diblock copolymer used as stabilizer in the dispersion polymerisation. In addition, the hydrophilic character of the spherical PDMA brush can be adjusted by changing the solution pH.

For the investigation of the particle location in the interface and the interface concentration, ellipsometric measurements at the water-air and water-dodecane interface were performed for different pH-values and temperatures. Difficulties in ellipsometry for this specific system are discussed and first results are presented.

[1] J. I. Amalvy, S. P. Armes, B. P. Binks, J. A. Rodrigues, and G-F. Unali, Chem. Commun., 1826 (2003)

CPP 30.40 Di 16:30 Poster TU D

Investigation of the Internal Structure of Polyelectrolyte Multilayers by means of Neutral Impact Collision Ion Scattering Spectroscopy — •Thomas Krebs, Gunther Andersson, and Harald Morgner — Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstrasse 2, 04103 Leipzig

The vertical ordering in polyelectrolyte multilayers of Polydiallyldimethylammonium (PDDA) chloride and Sodium polystyrenesulfonate with film thicknesses of 20 to 40 nm has been investigated by means of Neutral Impact Collision Ion Scattering Spectroscopy (NICISS). NICISS allows a model-independent evaluation of concentration depth profiles of all elements in the polyelectrolyte multilayer. By labeling certain polyelectrolyte layers with heavy atom (Ru) probes sufficient contrast has been obtained to visualize and quantify the distribution of these labeled polyelectrolytes throughout the film.

The effect of exposition of the samples to high temperatures and high salt concentrations has been investigated. An increased layer interdiffusion is observed with increasing temperature and increasing salt concentration.

The distribution of small counter ions in the film has also been investigated. PDDA has been deposited with either Chloride or Bromide as a counter ion. The depth profiles show that chloride is located exclusively at the outermost layer. On the other hand bromide is distributed throughout the whole film. The different behavior may be related to the different hydrophobicities of the two species.

CPP 30.41 Di 16:30 Poster TU D

Mechanisms of Protein Resistance in Oligo (Ethylene Glycol) Self-Assembled Monolayers: A Neutron Reflecitvity and FTIR Study — •M. Skoda[1], F. Schreiber[1], J. Willis[1], R. Jacobs[1], R. Dahint[2], M. Grunze[2] und M. Wolff[3] — [1]Phys. and Theor. Chemistry Laboratory, Univ. of Oxford, Oxford OX1 3QZ — [2]Angew. Phys. Chemie, Univ. Heidelberg, 69120 Heidelberg — [3]ILL, 38042 Grenoble-France

For the efficient development of custom designed oligo (ethylene glycol) (OEG) protein resistant coatings a thorough understanding of the underlying mechanisms leading to the repulsion of proteins in these self-assembled monolayers (SAMs) is necessary[1,2]. In this context [3] protein resistent OEG SAMs and their interactions with proteins in aqueous solutions have been studied in situ using neutron reflectivity (NR). Complementary data were taken using IR and optical spectroscopy. Sample parameters (temperature, ionic strength, pH and protein charge) have been varied to determine the values for the onset of the breakdown of the non-fouling properties. The NR data analysis was focused on the formation of a protein depleted zone in the proximity of the SAM/water interface. The shape of the concentration profile of the proteins was extracted from the data. Finally,a comprehensive discussion of the various control parameters influencing the protein resistance and the structure at the interface is attempted.

[1] Prime, K. L. et al., G. M.,Science,1991,252,1164;
[2] Schreiber, F., J. Phys.: Condens. Matter,2004,16,R881;
[3] Zheng, J. et al.,Langmuir,2004,20,893

CPP 30.42 Di 16:30 Poster TU D

Single Molecule Spectroscopy of Perylene Bisimide Derivatives and their Supramolecular Assemblies — •Erwin Lang[1], Hanna Engelke[1], Peter Osswald[2], Rainer Dobrawa[2], Frank Würthner[2], and Jürgen Köhler[1] — [1]Experimental Physics IV, University of Bayreuth — [2]Institute of Organic Chemistry, University of Würzburg

Self-assembly processes, starting from individual molecular building blocks and combining them to supramolecular structures of unbelievable variety, play a crucial role in life sciences. As a simple model system for self assembly we investigate pyridine-substituted perylene bisimide dyes, which form in the presence of cis-Pt(II) metal centres nanosized molecular squares.

Here we present a characterisation of the photophysical properties of the monomers and the molecular squares obtained by low-temperature single-molecule spectroscopy.

CPP 30.43 Di 16:30 Poster TU D

Polymer-induced transient networks in water-in-oil(w/o)-microemulsions — •Tinka Spehr, Thomas Blochowicz, Ahmed Sayeed, and Bernd Stühn — Technische Universität Darmstadt, Institut für Festkörperphysik, Hochschulstr. 8, 64289 Darmstadt

We study water in oil microemulsions which are dispersions of water droplets coated with a monolayer of surfactant in a continuous oil phase. Of particular interest for the present work is the system consisiting of water, n-decane and the anionic surfactant AOT, which we investigate by small-angle X-ray scattering (SAXS) and photon correlation spectroscopy (PCS). Below room temperature the structure of our one phase microemulsion is characterized by water droplets with a well defined radius in an oil matrix. In a former study of a complementary system (o/w-microemulsion with nonionic surfactant) the addition of a triblock copolymer led to the interconnection of the micelles. [1] In our case the polymer used is PEO(polyethylenoxide)-PI(polyisoprene)-PEO which has hydrophilic headgroups and a hydrophobic middle part.

We are monitoring the formation and structure of the network with SAXS to determine the structure factor and the domain form factor. Furthermore PCS is used to observe the dynamics of concentration fluctuations comprising the translational diffusion of the droplets and the relaxation of the network. Compared to the earlier study our system shows a remarkable increase of the viscosity at a much lower number of polymers per droplet. This effect is either caused by a higher degree of crosslinking or a longer lifetime of the junctions in our system.

[1] M. Schwab and B.Stühn, J. Chem. Phys. 14, 6461, (2000)

CPP 30.44 Di 16:30 Poster TU D

Equilibrium domain spacing and structure of PEO-PPO-PEO triblock copolymers studied by means of SAXS, DSC and OM — •Fajun Zhang and Bernd Stühn — Technische Universität Darmstadt, Institut für Festkörperphysik, D-64289 Darmstadt

Phase-separated morphology and domain structure of a series of PEO-PPO-PEO triblock copolymers (Pluronics) were studied. Phase separation was induced by crystallization of PEO block at the temperatures lower than the melting point. While in the melt state, PEO and PPO blocks are miscible, a disordered state with composition fluctuation was observed by SAXS. Upon crystallization of the PEO block, the amorphous PPO block was forced into the amorphous layer. The long-period and the thickness of crystalline phase were calculated from SAXS profiles, while the morphology and melting behavior were characterized by POM and DSC respectively. Both chain-extended and chain-folded crystalline phase could be formed depending on the relative length of PPO and PEO block, and the chain-folding structure could also be tuned by varying crystallization temperature. Equilibrium domain spacing was determined and compared to the results of mean-field theory. A detailed analysis of the SAXS profiles indicated that the phase-separated structure was not always formed by amorphous/mono-crystal alternating structure. An amorphous/bilayer-crystal structure was observed for samples with weight fraction of PEO less than 50 percent and crystallized at lower supercooling.

CPP 30.45 Di 16:30 Poster TU D

Wetting Morphologies in Triangular Grooves — •Krishnacharya Khare, Evgeny Gurevich, Bruce Law, Stephan Herminghaus, and Ralf Seemann — MPI for Dynamics and Self-Organization, D-37073 Göttingen

We have studied the wetting behavior of a various liquids in triangular grooves with chemically homogeneous walls. The length scale has been chosen to be small compared to the capillary length in order to avoid gravitational effects, but large enough for long range wetting forces (such as the van der Waals force) to be irrelevant. Droplets form elongated morphologies for contact angles smaller than 90 degree minus half the opening angle of the groove. For manipulating small amounts of liquids on that substrate (open microfluidics), we used electrowetting. We could vary the contact angle of the liquid on the substrate as a function of the applied Voltage. Filling and drainage behavior of these grooves were studied as a function of time and contact angle. In contrast to grooves with rectangular cross section, the liquid filaments in triangular grooves undergo an instability when being quenched from a filling to a non-filling situation. The liquid filament breaks up into isolated droplets with a preferred distance. The separation of the droplets depends upon the quench depth in a characteristic manner.

CPP 30.46 Di 16:30 Poster TU D

Photo- and Electrochemical Stability of Dye-Labelled Oligonucleotides Tethered to Au Surfaces — •Kenji Arinaga[1,2], Ulrich Rant[2], Marc Tornow[2], Shozo Fujita[1], Naoki Yokoyama[1], and Gerhard Abstreiter[2] — [1]Fujitsu Laboratories Ltd., 10-1 Morinosato-Wakamiya, Atsugi 243-0197, Japan — [2]Walter Schottky Institut, Technische Universitaet Muenchen, 85748 Garching, Germany

Fluorescence investigations represent a powerful and widespread method to study dye-labelled oligonucleotides tethered to surfaces. Recently, we have been introducing the dynamic electrical manipulation of short DNAs on a biased Au surface, employing optical measurements to probe the orientation of the surface grafted DNA strands [1]. While this technique opens many possibilities for fundamentals and applications, long-time stability is a crucial issue to carry out sophisticated studies.

In this contribution, we assess the photo- and electrochemical stability of the employed DNA layers under controlled substrate potentials. The beneficial influence of the metal surface in proximity to the dye on its photostability is elucidated. Further, the durability of the organic adlayer against varying substrate potentials is studied to achieve maximal manipulation efficiency along with negligible sample degradation.

As a result, it is demonstrated that electro-optical investigations of surface grafted DNA layers can be conducted with extraordinary long-time stability and persistent functionality.

[1] U. Rant et al., Nano Letters (in press)

CPP 30.47 Di 16:30 Poster TU D

Conductive Polymers in Nanotemplates — •Radim Křenek[1], Alexander Sidorenko[1], Věra Cimrová[2], and Manfred Stamm[1] — [1]Leibniz Institut für Polymerforschung e.V., Hohe Str. 6, 01069 Dresden, Germany — [2]Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, Heyrovsky Sq. 2, 162 06 Prague 6, Czech Republic

We report on synthesis of conductive polymers in block copolymer (BC) nanotemplates, polyaniline (PANI) and poly(3,4-ethylenedioxythiophene) (PEDOT). The nanotemplates are based on self-organization of poly(styrene-block-4-vinylpyridine) (PS-PVP) with low molecular additive (LMA). Thin porous nanotemplates were prepared by coating from solution of PS-PVP+LMA and selective washing of LMA from the film [1]. The cylindrical pores of 8 nm in the diameter are ordered in a hexagonal lattice (24 nm in the period) as determined from AFM in tapping mode. PANI and PEDOT were synthesized in the porous nanotemplates electrochemically. Presence of the polymers in the nanopores was proven using uv-vis spectrophotometry, atomic force microscopy (AFM) and ellipsometry. Electrical properties of the devices (glass/ITO/PANI/Al and glass/ITO/BC+PANI/Al) were studied. Current-voltage characteristics of the devices are compared and discussed.

[1] A. Sidorenko, I. Tokarev, S. Minko, M. Stamm: J. Am. Chem. Soc. 125 (2003) 12211

CPP 30.48 Di 16:30 Poster TU D

Chain stratification and anisotropy in polyelectrolyte multilayers — •Abbass Kazemi[1,2] and Monika Schönhoff[1,2] — [1]Institut für Physikalische Chemie, WWU Münster, Corrensstr.30, D-48149 Münster — [2]Max-Planck-Institut für Kolloid- und Grenzflächenforschung, D-14424 Golm

Polyelectrolyte multilayers (PEMs) prepared by self-assembly form materials in which the chains are adsorbed in 2-dimensional monomolecular layers. However, structural investigations show a strong interdigitation of adjacent layers, which contradicts the picture of 2-dimensional chains. The chain conformation is studied here by extracting order parameters (S2) of the out-of-plane orientation distribution of polymer segments, i.e. the out-of-plane anisotropy, from UV linear dichroism. Polystyrene sulfonate (PSS) is employed as the anionic component, while the chain stiffness of the cationic component as well as the salt concentration and the number of layers are varied. The results show that the side groups are preferentially oriented in the direction of the surface normal. With increasing layer number, the order parameter decreases for most PEM systems, and reaches a plateau. The salt-dependence is in agreement with existing models of the chain conformation in multilayers. An interesting point is that even for large layer numbers and high salt concentration, no isotropic order is obtained. The order parameters reach values around 0.35, well above 0, implying that the chain conformation is rather 2-dimensional, with well-ordered segments preferentially oriented along the surface normal. This new result clearly contradicts existing views of PEMs as locally isotropic complexes.

CPP 30.49 Di 16:30 Poster TU D

Polymer – surfactant interactions: Effect of surfactant concentration on polymer conformation and aggregation size — •J.B. Stanislaus[1], H. Zettl[1], J. Crassous[2], L. Li[2], O. Korenberg[3], M. Gottlieb[3], M. Ballauff[2], and G. Krausch[1] — [1]Physical Chemistry II, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth. — [2]Physical Chemistry I, Universität Bayreuth, Universitätstraße 30, 95440, Bayreuth. — [3]Department of Chemical Engineering, Ben–Gurion University of the Negev, Israel.

Association between polymers and surfactants has drawn much attention in the last decades. Mixed aggregates are formed already at low surfactant concentration, and can change the solution properties dramatically. This in turn affords a variety of industrial applications (cosmetics, paints,. etc). In this work we study a system containing an anionic surfactant sodium dodecyl sulphate (SDS) and a non ionic polymer methylcellulose (MC) in water. Fluorescence correlation spectroscopy(FCS) is used to study the dynamics of the aggregates. We are able to follow the change of the solution properties over a wide concentration range of both polymer and surfactant. The maximum aggregation of MC and SDS is linearly dependent on MC concentration. The results are compared to Small Angle X-ray Scattering (SAXS) and rheology measurements.

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pH-Dependent Aggregation Behaviour of Polypeptide-Polybutadiene Block-Copolymers in Aqueous Solution — •Reinhard Sigel, Magdalena Losik, and Helmut Schlaad — Max-Planck-Institut of Colloids and Interfaces, Am Mühlenberg 1, D-14476 Golm

Block-Copolymers composed of 1,2-polybutadiene-*block*-poly(L-lysine) (PB-*b*-PL) form aggregates in saline aqueous solution because of the insoluble PB-block. The soluble PL block is changed from a random coil to a helix by varying the solution pH value. This conformational switching is expected to change also the aggregation properties of the polymer. Unfortunately, dynamic light scattering measurements show a strong and curved dependency of the diffusion constant on the scattering angle, which renders a standard data analysis impossible. The phenomena is interpreted as an inhomogeneous distribution of the aggregates in the highly dilute solution, which is caused by weak but long range attractive interactions. In regions with high concentration, the effect of the structure factor and the hydrodynamic mobility function on the diffusion become important. A data analysis including these effects is discussed.

CPP 30.51 Di 16:30 Poster TU D

Free standing liquid filaments: structure, mechanical and electrical properties — •Alexandru Nemes[1], Alexey Eremin[1], Mario Schulz[2], Ralf Stannarius[1], Hajnalka Nádasi[3], and Wolfgang Weissflog[3] — [1]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik — [2]LKA Sachsen-Anhalt — [3]Martin-Luther-Universität Halle, Institut für Physikalische Chemie

Simple liquids cannot form filaments with lengths exceeding their diameter by more than a factor of π because of the Rayleigh-Plateau instability. However, there are examples of stable filaments with slenderness ratios exceeding 1000, formed by complex fluids, e.g. bent-core liquid crystals.

Similar fibers can be found in nature, for example, spider silk undergoes a mesophase transition in the spinning process.

In our work, we present the results of experiments performed on several bent-core liquid crystalline materials which form filaments with radii of few micrometers, and axial extension of several millimeters.

In particular, we report mechanical, AFM, X-Ray and optical measurements that reveal the internal structure, dynamics and mechanical and electrical properties of these filaments.

CPP 30.52 Di 16:30 Poster TU D

Generation and purification of single-wall carbon nanotubes from alcohol and their characterization — •D. Malsch, M. Hofmann, R. Brunner, M. Eremtchenko, R. Öttking, S. Krischok, and J.A. Schaefer — TU Ilmenau, Institut für Physik und Zentrum für Mikro- und Nanotechnologie, Postfach 100565, 98684 Ilmenau

Since the discovery of carbon nanotubes in 1991 by S. Iijima, this new form of elemental carbon has arisen much research interest. Due to their small dimensions and unique mechanical and electronic properties, one can imagine many possible applications in micro- and nanotechnology

and other technological areas.

The growth of carbon nanotubes has been investigated in detail during the last ten years. Many factors have to be considered like yield, purity, quality and scalability. Here, the setup of an alcohol CVD according to Maruyama et al for the generation of single-wall carbon nanotubes is presented. Advantages of this setup are its simple and low-cost construction, its easy scalability and its safe operation while providing good growth results.

Growth parameters, catalyst preparation and purification methods are optimized for the yield and quality of single-wall carbon nanotubes. The characterization of this material with Raman spectroscopy and electron microscopy as well as surface-specific methods (photo electron spectroscopy and electron energy loss spectroscopy) has been applied.

CPP 30.53 Di 16:30 Poster TU D

Elekromechanische Eigenschaften von zellulären Polymerfolien — •Mario Dansachmüller, Johann Georg Leonhartsberger, Reinhard Schwödiauer, Simona Bauer-Gogonea und Siegfried Bauer — Abteilung Physik weicher Materie, Inst. f. Experimentalphysik, J. Kepler Universität Linz, 4040 Linz, Austria

Zelluläre Polymere mit intern geladenen geschlossenen Zellen weisen starke piezoelektrische Effekte auf, die für Sensor- und Aktoranwendungen von Interesse sind. Die Größe der internen Hohlräume kann durch einen speziellen Expansionsprozess gezielt eingestellt werden. Dabei wird das Polymergefüge mit Gas, z.B. mit Stickstoff oder Kohlendioxid unter hohem Druck gesättigt. Bei nachfolgender rascher Druckverringerung wird die Polymerfolie kontrolliert expandiert, anschließend wird die Struktur fixiert bei erhöhter Temperatur. Der Expansionsprozess wird on-line durch Kapazitätsmessungen der Folie verfolgt. Die mechanischen Eigenschaften der Folien werden ebenfalls durch kapazitive Messungen an geladenen Folien verglichen. Mit diesem Verfahren können die elektromechanischen Eigenschaften zellulärer Polymere optimiert werden.

CPP 30.54 Di 16:30 Poster TU D

Präparation und Charakterisierung von mesoporösem Zinndioxid für Gassensoranwendungen — •Thorsten Wagner[1], Michael Tiemann[2], Michael Fröba[2] und Claus-Dieter Kohl[1] — [1]Justus-Liebig-Universität, Institut für Angewandte Physik, Gießen — [2]Justus-Liebig-Universität, Institut für Anorganische und Analytische Chemie, Gießen

Wir untersuchten Synthese und Gassensoreigenschaften von mesoporösem Zinndioxid, welches auf verschiedene Arten hergestellt wurde:

In einem Ansatz wurden supramolekulare Aggregate organischer Amphiphile als Strukturdirektoren (Endotemplating) verwendet. Um diese baut sich das anorganische Netzwerk aus dem Precursor, $SnCl_2$, auf.

Eine Alternative ist die Herstellung durch Exotemplating. Hierbei wird ein geordneter, poröser Festkörper als Templat verwendet. In diesen wird in mehreren Schritten ein anorganischer Precursor eingelagert und anschließend durch eine Temperaturbehandlung in das Oxid überführt. Im letzten Schritt wird das Templat entfernt.

Die spezifischen Oberflächen und Porendurchmesser der Materialien wurden mit Hilfe von Stickstoffphysisorption bestimmt. Zur Strukturbestimmung wurden Röntgenpulverdiffraktometrie und TEM eingesetzt. Des weiteren wurde ein Vergleich mit Zinndioxidpulver, das mit einem Sol-Gel-Verfahren hergestellt wurde, durchgeführt.

Die Porendurchmesser der synthetisierten Materialien liegen bei 4 nm und die spezifischen Oberflächen bei mehr als $150\frac{m^2}{g}$ (kommerziell erhältliches Zinndioxidpulver ca. $40\frac{m^2}{g}$).

CPP 30.55 Di 16:30 Poster TU D

Negatively Charged Water Dispersible Prussian Blue Nanoclusters and Decoration of Single Polycation Chains and Carbon Nanotubes — •Ganna Gorodyska[1], Vera Bocharova[1], Anton Kiriy[1], Paul Simon[2], Manfred Stamm[1], Xudong Lou[3], Francois Stoffelbach[3], Christophe Detrembleur[3], and Robert Jérôme[3] — [1]Leibniz-Instituts für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]Center for Education and Research on Macromolecules (CERM), University of Liege, Sart-Tilman, B6, 4000 Liege, Belgium

A simple method is reported in this work for the preparation of charge-stabilized Prussian Blue nanocrystals of readily adjustable size. They have been purified by addition of non-solvents and redispersed in water without aggregation. PB nanocrystals have been electrostatically arranged along single polycation chains adsorbed onto flat surfaces or along carbon nanotubes precoated by a polycation. In the latter case, carbon nanotube-polyelectrolyte-Prussian Blue hybrids are formed, that might be useful materials for the manufacture of electrooptical devices or mechanically robust ion-sieving membranes.

CPP 30.56 Di 16:30 Poster TU D

Rotational Dynamics of Nonrigid Biomolecules in Solution: Influence of the Bead–Bead Interactions. — •Alexander Uvarov and Stephan Fritzsche — Universität Kassel, D–34132 Kassel, Germany

During the past decade, a large number of experiments and molecular dynamic simulations have been carried out in order to describe the statical and the dynamical properties of biomolecules. An alternative treatment of biomolecules is presided by statistical methods if they are described in terms of their molecular subsystems, the so–called beads of the macromolecule[1].

In this contribution we investigate the effects of the bead–bead interaction potential on the orientation and relaxation processes of the biomolecules immersed in the solvent. We present and discuss the explicit expression for the configuration–space distribution function of a *non*–rigid molecule which is immobilized on a surface. These function contains all the information about the interaction among the beads as well as the effects from the surrounding solvent particles and from the surface. Detailed computations for the distribution functions and the rotational diffusion coefficient of the macromolecule have been carried out for HOOKEAN, FENE, and a DNA–type bead–bead interaction. Results from our theory are then compared with other computations which are based on a *rigid–rod model* of the macromolecules[2].

[1] A. Uvarov and S. Fritzsche, Macrom. Theory and Simul., **13**, 241 (2004); A. Uvarov and S. Fritzsch, Chem. Phys. Letters, (submitted)

[2] A. Uvarov and S. Fritzsche, J. Chem. Phys. **121**, 6561, (2004)

CPP 30.57 Di 16:30 Poster TU D

Nonlinear Dynamics of Vibrational Excitons in Polypeptides — •Dmitry Tsivlin and Volkhard May — Institut für Physik, Humboldt Universität zu Berlin, Newtonstraße 15, D-12489 Berlin, Germany

Ultrafast infrared spectroscopy of polypeptides and small proteins attracted a lot of interest in recent years. Concentrating on high-frequency vibrations of the peptide unit, such as amide I modes, delocalization and relaxation could be observed mainly in the framework of multidimensional spectroscopy. In Ref. [1] the observation of a self–trapped vibrational state in the helical conformation of poly–γ–benzyl–L–glutamate has been reported using recent studies on two–vibron bound states [2]. By introducing the concept of *adiabatic excitons* we reexamine these states of the helix. Diagonalizing the full Hamiltonians responsible for the presence of a different number of peptide group excitations we can study various mechanisms leading to the self–trapping of, e.g. the amide I or N–H mode. Relaxation channels for their deexcitation are also discussed. Some preliminary results on a mixed quantum–classical description of the formation and decay of self–trapped states are reported.

[1] J. Edler, et al., Phys. Rev. Lett. **93**, 106405 (2004)

[2] V. Pouthier, Phys. Rev. E **68**, 021909 (2003)

CPP 30.58 Di 16:30 Poster TU D

Dynamical relaxation of copolymeric structures — •Cristian Satmarel[1], Alexander Blumen[1], Andrei Gurtovenko[2,3], and Christian von Ferber[1] — [1]Theoretische Polymerphysik, Universitaet Freiburg, Hermann-Herder-Str. 3, 79108 - Freiburg, Germany — [2]Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoi Prospect 31, V.O., St. Petersburg, 199004, Russia — [3]Laboratory of Physics and Helsinki Institute of Physics, Helsinki University of Technology, P.O. Box 1100, FIN-02015 HUT, Finland

We treat the dynamics of copolymeric structures with heterogeneity in the mobility of the beads using the Rouse model. The structures that we treat are alternating copolymer chains and regular lattice networks built from these, dendrimers with alternating generations, as well as branched polymers synthesized by end-linking star-like units. We show the effects of alternating mobility of the beads. These effects are well seen in the mechanical relaxation quantities, such as the storage and the loss moduli. The dynamics of the end-linked star polymer structures combines the relaxation of the star arms (spacer chains) and the branching units. We analytically separate these two processes and map the eigenmode spectrum of a homogeneous system to that of a system with spacers. When the spectrum of the homogeneous system is known analytically,

this allows for a full analytic solution. We discuss also the important effects connected to the length and mobility of the spacers. [Refs: C. Satmarel, A.A. Gurtovenko, A. Blumen, Macromolecules, (2003), vol.36, 486; Macromol. Theory Simul., (2004), vol.13, 487.]

CPP 30.59 Di 16:30 Poster TU D

Transport and diffusion properties of macromolecules in solution — •Alexander Uvarov and Stephan Fritzsch — Universität Kassel, D–34132 Kassel, Germany

Accurate dynamical studies on macromolecules in solution are still a challenge for modern DNA and protein research. During the past decade, therefore, a large number of experiments and molecular dynamic simulations(MDS) have been carried out in order to understand the diffusion properties of macromolecules, i.e. their translational and rotational motion, if immersed into a solution. An alternative treatment of biomolecules is presided by statistical methods if they are described in terms of their molecular subsystems, the so–called beads, and if all information about the influence of the solvent on the dynamics of the macromolecule is incorporated to the friction tensors of the macromolecule.

In this contribution we utilize a recently described[1] the explicit expression for the friction tensors, in order to calculate their diffusion coefficient as function of the mass ratio of the molecules, relative to the mass of the solvent particles. In addition, we also study the effect of the transition between slip and stick boundary conditions by calculating the boundary condition coefficient of the macromolecule immersed in the solvent for different mass ratios as well as different bead–solvent potentials. The results from our semi–phenomenological theory are found to compare very well with MDS works over a wide range of mass ratios and at quite different temperatures and viscosities of the solvent[2].

[1] A. Uvarov and S. Fritzsche, Macrom. Theory and Simul., **13**, 241 (2004); [2] A. Uvarov and S. Fritzsch, Chem. Phys. Letters, (submited)

CPP 30.60 Di 16:30 Poster TU D

Dewetting of confined polymer films — •E. Bauer and P. Müller-Buschbaum — TU-München, James-Franck-Str.1, 85747 Garching

Dewetting is of major interest in many applications such as coatings and dielectrics. We investigated the dewetting behavior of ultra-thin (confined) polystyrene films on top of differently cleaned Si-substrates by exposure to heat load. The samples were probed by AFM and GISAXS. We found out that the dewetting is modifed upon the type of cleaning procedure applied. Time scales as well as final states are different. The time dependent hole growth differs from the common slip or non-slip condition. By cleaning a thickness change of the native oxide layer is reported which alters the wall potential. An analysis of the wall potential leads to a relation of the differing time scales to binodal and spinodal mechanisms. Characterizing the near equilibrium states by an analyse of the contact angle between substrate and polymer again showed the importance of short range contributions in the wall potential. By cleaning, the physics of the system is seriously affected [1, 2].

[1] P.Müller-Buschbaum, Euro. Phys. J. E 12, 443 (2003)
[2] E.Bauer, P.Müller-Buschbaum, to be published

CPP 30.61 Di 16:30 Poster TU D

Sol Molecular Weight Distribution of Ion irradiated Polystyrene — •Ralf Delto and Rüdiger Brenn — Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str.3, 79104 Freiburg

Irradiation of polymers with high energetic ions results in a change of molecular weight distribution and produces gel and sol fractions by breaking of chains and formation of crosslinks.

While the crosslinked chains can form an insoluble network (gel), there remains a soluble part (sol). The distribution of molecular weights in the sol depends on the applied ion dose and can hence be controlled experimentally. We calculate the M_w distributions with statistical methods and with numerical simulations.

Measurements are performed on polystyrene (PS) thin films. We use 1 MeV protons for irradiation. The irradiated sol (dPS) diffuses into a polymer network (PS) while heating above T_g. As the diffusion constant depends on the molecular weight, the different species diffuse unequally fast. Thus the diffusion profiles contain information about the abundance of chains of different degrees of polymerisation in the sol. Diffusion depths profiles for the deuterated component (sol) are determined with ^{3}He nuclear reaction analysis.

CPP 30.62 Di 16:30 Poster TU D

Freies Volumen in Membranpolyimiden: Variation der Diamin-Geometrie — •Jan Kruse[1], Jörn Kanzow[1], Klaus Rätzke[1], Franz Faupel[1], Matthias Heuchel[2], Jörg Frahn[2] und Dieter Hofmann[2] — [1]Universität Kiel, Kaiserstr. 2, 24143 Kiel — [2]GKSS-Forschungszentrum, Kantstr. 55, 14513 Teltow

Die Gastrennung mit Polymermembranen besitzt zunehmende Bedeutung für industrielle Anwendungen. Menge und Verteilung des freien Volumens bestimmen maßgeblich Transport- und Trennungseigenschaften. In dieser Arbeit werden einerseits die geometrischen Eigenschaften des erreichbaren freien Volumens direkt aus MD-Simulationen durch Abtasten mit einer "virtuellen Tracerkugel" bestimmt [1]. Andererseits wird mit der Positronenlebensdauerspektroskopie (PALS) der mittlere Lochradius experimentell bestimmt [2]. Variationen der Struktur des Diaminmonomers führen zu einer Änderung des freien Volumens. Ferner wird die Vergleichbarkeit von Simulationsergebnissen und PALS-Messungen diskutiert [3].

[1] E. Schmidtke et al. J. Mol. Graphics and Modelling, 22, 309 (2004).
[2] C. Nagel et al. Macromolecules, 33, 2242 (2000).
[3] J. Kruse et al. Macromolecules, in preparation

CPP 30.63 Di 16:30 Poster TU D

Lithium Diffusion in the 2D Fast Ion Conductor *h*-$Li_{0.7}TiS_2$ Probed by Nuclear Magnetic Relaxation and Two-Time ^{7}Li Stimulated-Echo NMR — •Martin Wilkening, Wilfried Küchler, and Paul Heitjans — Universität Hannover, Institut für Physikalische Chemie und Elektrochemie

Classical spin-spin and spin-lattice relaxation NMR in the laboratory as well as in the rotating frame on the one hand and stimulated-echo NMR on the other hand are used for the first time for a comprehensive investigation of Li diffusion in hexagonal *h*-$Li_{0.7}TiS_2$. Combining these different techniques the same 2D diffusion process in layered $Li_{0.7}TiS_2$ was probed over a dynamic range of almost 10 orders of magnitude with jump rates ranging from $1{\cdot}10^{-1}$ s^{-1} to $7.8{\cdot}10^{8}$ s^{-1} (148 – 510 K). Whereas Li jump rates in the GHz to kHz range were probed by recording diffusion induced spin-lattice relaxation rates in the laboratory and rotating frame, ultra-slow Li jumps in the kHz to sub-Hz range were detected directly by recording mixing-time dependent two-time spin-alignment echoes. Taken together, the jump rates from the different methods obey the same Arrhenius behaviour with an activation energy of 0.41(1) eV and a preexponential factor of $6.3(1) \cdot 10^{12}$ s^{-1}.

CPP 30.64 Di 16:30 Poster TU D

Anisotropy of electron spin diffusion in organic quasi-1D-conductors — •Armin Warth, David Saez de Jauregui, Stefan Matejcek, and Elmar Dormann — Physikalisches Institut, Universität Karlsruhe(TH),

The organic conductors $(Fluoranthen)_2PF_6$ and $(Perylen)_2AsF_6 \times$ 2/3 THF belong to the family of the so called arene radical cation salts and provide good model systems for the investigating the one-dimensional electron dynamics. Like other representatives of the organic quasi-1D-conductors a Peierls-transition can be observed in both conductors but at different temperatures.

Using X-band-pulse-ESR techniques with optimized static field gradients the electron spin diffusion was examined for different orientations and a broad temperature regime below and above the semiconductor-metal phase transition. These analyzes were focused on the determination of the electron spin motion perpendicular to the molecular stacking axis *a*, where the diffusion seems to be dominated by a conduction electron hopping process.

The results show the highly anisotropic character of the systems comparing parallel and perpendicular to stack diffusion. By irradiating a fluoranthen crystals with high energetic protons, the concentration of localized paramagnetic defects could be increased and the anisotropy decreased by about two orders of magnitude.