

CPP 9: POSTERS Single Molecules, Biopolymers, Membranes

Time: Monday 16:45–19:00

Location: Poster A

CPP 9.1 Mon 16:45 Poster A

Quantification of singlet-singlet annihilation in an acceptor-donor-acceptor compound at the single molecule level — ●BURKHARD FÜCKEL¹, GERALD HINZE¹, FLORIAN DIEHL¹, FABIAN NOLDE², KLAUS MÜLLEN², and THOMAS BASCHÉ¹ — ¹Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Jakob-Welder-Weg 11, 55099 Mainz, Germany — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We have investigated a new multichromophoric compound consisting of a central peryleneimide donor (D) chromophore and two terryleneimide acceptor (A) chromophores adjacent to it (A-D-A). After electronic excitation of the donor chromophore, energy is rapidly transferred to the acceptor chromophores. Time-resolved measurements by means of optical single molecule spectroscopy revealed that singlet-singlet annihilation (SSA) takes place upon excitation of both acceptor chromophores.

We quantitatively determined the rate of the SSA process at the single molecule level. Our approach combines the detection of photon arrival time coincidences with Monte Carlo simulations. On average the SSA rate is found to be two to three times faster than the fluorescence lifetime of terryleneimide.

CPP 9.2 Mon 16:45 Poster A

Gold Nanoparticles Decorated with Oligo(ethylene glycol) Thiols: The Effect of Salt Nature on the Stability of Colloid-Protein Mixtures — ●FAJUN ZHANG¹, MAXIMILIAN W. A. SKODA^{1,2}, ROBERT M. J. JACOBS², STEFAN ZORN¹, RICHARD A. MARTIN³, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — ²CRL, University of Oxford, UK — ³Department of Physics, University of Bath, UK

The stability of mixtures of oligo(ethylene glycol) (OEG) thiol self-assembled monolayer protected gold colloids and globular proteins in solution, depends strongly on the nature of added salts. UV-vis spectroscopy was used to study the stability of the mixtures by monitoring the time dependence of the flocculation [1]. It was shown that the OEG-protected gold colloid solution is stable in the presence of NaCl, NaSCN, MgCl₂, but loses its stability on addition of Na₂SO₄. In the mixtures of colloid and protein, the colloids lose their stability and form aggregates upon adding protein above a critical concentration, c^* , due to the depletion effect [1]. Adding NaCl or Na₂SO₄ to the mixtures enhances the colloid aggregation; NaSCN stabilizes the solution, and MgCl₂ results in a long induction time before aggregation. The observed salt nature effects follow the “Hofmeister series” and are discussed based on the salting-in or salting-out effect as well as the ion-absorption effect. The salt nature effect is planned to be further studied by SAXS. [1] F. Zhang, et al., *J. Phys. Chem. B* 2007, 111, 251. *J. Phys. Chem. A* 2007, DOI: 10.1021/jp074293v. *Euro. Biophys. J.* Submitted.

CPP 9.3 Mon 16:45 Poster A

Blinking induced bleaching and recovery of organic dyes in polymer materials — ●INES TRENKMANN, JÖRG BRABANDT, JÖRG SCHUSTER, and CHRISTIAN VON BORCZYKOWSKI — TU Chemnitz, Institut für Physik, 09107 Chemnitz

Fluorescence intermittency, usually referred to as blinking, is a common feature of individual emitters embedded into or close to dielectric materials such as polymers or silicon oxides [1]. If the photoluminescence from ensembles of emitters is observed under conditions similar to single emitter studies, blinking processes lead to a reversible change of the intensity, which is in most cases a decrease of intensity [2]. Such reversible intensity decays and its recovery have been studied by us for ensembles of different dye/polymer systems. Our preliminary results show, that the kinetics of the fluorescence recovery is rather a function of the matrix than of the emitter. While fluorescence recovery of dyes in PVA occurs on a time scale of seconds it takes several hours to days in polystyrene. Based on those findings and recent publications [1] the model of blinking as a process of ejecting and trapping of charges in dielectric materials gains further evidence. In conclusion, we suggest to use blinking *vice versa* as a probe for charge trapping in dielectric properties. Our results show, that blinking phenomena can be studied easily on the ensemble level by bleaching and recovery experiments.

[1] F. Cichos, C. von Borczykowski, M. Orrit: *Curr. Op. Coll. Interf.*

Sc. 12 (2007), 272

[2] J. Brabandt, J. Schuster, C. von Borczykowski: *J. Luminescence* 127 (2007), 224

CPP 9.4 Mon 16:45 Poster A

New NIR fluorophores for single molecule microscopy — GEORG M. FISCHER, MARTIN WINTERHALDER, MAGNUS ISOMÄKI-KRONDAHL, ANDREAS ZUMBUSCH, and ●M. YAVUZ YÜCE — Department Chemie, Universität Konstanz, Fach M722, D-78457 Konstanz

Excitation in the near infrared (NIR) generally leads to lower background signal in single molecule experiments. For this reason, strongly fluorescent chromophores which absorb and emit in the NIR are highly desirable for such applications. According to the energy gap law, however, most fluorophores will only exhibit very weak NIR fluorescence emission. Here we present a new class of dyes based on diketopyrrolopyrroles. At absorption wavelengths of up to 800 nm, these dyes still exhibit fluorescence quantum yields of more than 50%. We have characterized a broad variety of derivatives both on the ensemble and on the single molecule level.

CPP 9.5 Mon 16:45 Poster A

Measuring distance fluctuations by single pairs of gold nanoparticles — ●MIRIAM WÄHNERT¹, ROMY RADÜNZ², and FRANK CICHOS³ — ¹Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig — ²Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig — ³Molecular Nanophotonics Group, University Leipzig, 04103 Leipzig

Single Molecule fluorescence resonance energy transfer (SMFRET) measures distance changes. This is heavily applied in biophysical studies. In combination with time resolved time tagged fluorescence detection it even allows the study of the dynamics of conformational fluctuations. However, the distance fluctuations accessible are limited to a range up to about 10 nm. Further, the technique suffers often from fluorescence blinking or bleaching of either donor or acceptor of the energy transfer dye couple.

We report on experiments, which employ the plasmon coupling between two gold nanoparticles to monitor distance fluctuations. The plasmon coupling of two gold particles is visible at distances up to a few 10 nm. Therefore it measures distance fluctuations on a much longer lengthscale than SMFRET. The interaction of the two plasmon oscillations shifts the extinction spectrum to longer wavelength. An optical signal off resonance of the single particle resonance is a measure for the particle distance. We use a photothermal detection technique to monitor the distance fluctuations between very small particles that are difficult to detect by optical scattering. First experimental results will be presented together with a numerical analysis of the technique.

CPP 9.6 Mon 16:45 Poster A

Investigations of single quantum dot (QD) blinking via Fluorescence Correlation Spectroscopy (FCS) — ●NICOLE AMECKE and FRANK CICHOS — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

The intermittency of QD fluorescence (blinking) is a well known, intensively studied, but still not fully understood phenomenon. Control over this peculiarity is strongly desired for many applications of QDs as reliable light sources. This however remains still a fair wish and needs deeper understanding of the underlying processes. The observed dark states are supposed to result from ionization processes, where one charge is ejected from the QD into localized states of the surrounding medium. Auger processes, enabled by the remaining charge, will then inhibit photon emission until neutralization. The durations of dark (charged) as well as bright (neutral) periods are found to obey power law statistics, which can be understood to result from a tunneling process of the charge to and from a wide distribution of trap states in the matrix. This explanation holds for a solid matrix while deviations in liquid matrices can be expected. In ensemble investigations effects of blinking simply result in lower emission intensity. FCS, however, offers a method to investigate blinking of QDs in solution. When keeping the detection volume small via confocal spectroscopy, the diffusion of single emitters through the focus can be investigated, obtaining diffusion properties, but also blinking effects. We find that both, shape and contrast, of the correlation function depend on the excitation power.

This leads to an apparent concentration change as deduced by FCS.

CPP 9.7 Mon 16:45 Poster A

Kinetics of TmHU binding to DNA as observed by optical tweezers — ●MATHIAS SALOMO, CAROLIN WAGNER, ULRICH KEYSER, and FRIEDRICH KREMER — Linnéstraße 5, 04103 Leipzig

The kinetics of binding for the histone-like protein TmHU (from *Thermotoga maritima*) to DNA is analyzed on a single molecule level by use of optical tweezers. For the reaction rate a pronounced concentration-dependence is found with an "all or nothing-limit" which suggests the cooperative nature of the binding-reaction. By analyzing the statistics of mechanically induced dissociation-events of TmHU from DNA multiple reaction sites are observed to become more likely with increasing TmHU concentration. This is interpreted as a hint for a secondary organizational level of the TmHU/DNA complex. The reaction rate of TmHU binding to DNA is remarkably higher than that of the HU protein from *Escherichia coli* which will be discussed.

CPP 9.8 Mon 16:45 Poster A

Higher order laser modes as a tool to determine single-molecule orientation in an optical microresonator — ●RAPHAEL GUTBROD, ANNA CHIZHIK, DMITRY KHOPTYAR, and ALFRED JOHANN MEIXNER — University of Tübingen, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 8, 72076 Tübingen (Germany)

Subwavelength optical microresonators show great potential as a platform for single-photon emitting sources and sensors on the nano-scale. Due to modification of the optical state density inside the microresonator the emission properties of single molecules can be strongly modified, which includes spectral and spatial redistribution of the spontaneous emission as well as enhancement and inhibition of the spontaneous emission rate due to the Purcell-effect [1].

A recently developed technique for determination of single-molecule orientation is based on excitation with azimuthally and radially polarized doughnut laser modes. Analysing the single molecular excitation patterns with confocal microscopy allows one to determine the orientation for many molecules from one scan image.

Using a novel microresonator designed in our group we investigate the excitation patterns of fluorescent beads with these laser modes aiming at a better understanding of the cavity electrodynamics. This is a crucial point for optimal cavity design which may open a perspective for new integrated nano-optical sensing.

[1] M. Steiner, F. Schleifenbaum, C. Stupperich, A. V. Failla, A. Hartschuh, A. J. Meixner. *ChemPhysChem* 2005, 6, 2190

CPP 9.9 Mon 16:45 Poster A

N-V center in diamond as spin-selective sensor — ●BERNHARD GROTZ, GOPALAKRISHNAN BALASUBRAMANIAN, INAM MIRZA, FEDOR JELEZKO, and JÖRG WRACHTRUP — 3. Physikalisches Institut, Universität Stuttgart, Germany

Due to its biocompatibility and chemical stability, diamond is a promising candidate for biological applications. In particular fluorescent properties of N-V colour centers in diamond have attracted interest because of unlimited photostability [1]. We show the concept and first experiments how such colour centers can be used as a sensor for biomolecules absorbed on diamond surfaces. Since N-V centers are paramagnetic, their fluorescence can be employed as spin-selective sensor.

[1] A. Gruber et al., *Science* 276, 2012 (1997)

CPP 9.10 Mon 16:45 Poster A

A detailed theoretical analysis of the optical spectra of the prototype molecules tetracene and rubrene — ●TARAS PETRENKO, OLGA KRYLOVA, MORITZ SOKOLOWSKI, and FRANK NEESE — Institute for Physical and Theoretical Chemistry, Bonn University, Wegelerstrasse 12, 53115 Bonn, Germany,

Tetracene and rubrene are two prototype fluorescent molecules which are presently intensively studied. Interestingly, both molecules exhibit the same fluorescent backbone. However, due to electric repulsion between the phenyl groups, the backbone of rubrene is twisted, whereas it is planar for tetracene. Optical spectroscopy reveals that the $S_0 \rightarrow S_1$ transition in rubrene is redshifted with respect to tetracene by $\sim 2000 \text{ cm}^{-1}$ and that rubrene exhibits a considerably larger Stokes shift. In order to unravel the physical effect responsible for these differences we have performed normal coordinate analysis and frequency calculations using density functional theory in conjunction with linear response time-dependent density functional theory energy scan calcu-

lations. This yielded dimensionless normal coordinate displacements of the excited-state origin that were employed to calculate and fit the vibrational finestructure in absorption and fluorescence spectra. The analysis reveals that the $\sim 2000 \text{ cm}^{-1}$ red shift of 0-0 vibronic band of rubrene relative to tetracene is mainly caused by the inductive effect of the phenyl substituents that leads to destabilization of the donor MO. (Funded by the DFG research unit 557 and the university of Bonn)

CPP 9.11 Mon 16:45 Poster A

A detailed theoretical analysis of the optical spectra of the prototype molecules tetracene and rubrene — ●TARAS PETRENKO, OLGA KRYLOVA, MORITZ SOKOLOWSKI, and FRANK NEESE — Institute for Physical and Theoretical Chemistry, Bonn University, Wegelerstrasse 12, 53115 Bonn, Germany,

Tetracene and rubrene are two prototype fluorescent molecules which are presently intensively studied. Interestingly, both molecules exhibit the same fluorescent backbone. However, due to electric repulsion between the phenyl groups, the backbone of rubrene is twisted, whereas it is planar for tetracene. Optical spectroscopy reveals that the $S_0 \rightarrow S_1$ transition in rubrene is redshifted with respect to tetracene by $\sim 2000 \text{ cm}^{-1}$ and that rubrene exhibits a considerably larger Stokes shift. In order to unravel the physical effect responsible for these differences we have performed normal coordinate analysis and frequency calculations using density functional theory in conjunction with linear response time-dependent density functional theory energy scan calculations. This yielded dimensionless normal coordinate displacements of the excited-state origin that were employed to calculate and fit the vibrational finestructure in absorption and fluorescence spectra. The analysis reveals that the $\sim 2000 \text{ cm}^{-1}$ red shift of 0-0 vibronic band of rubrene relative to tetracene is mainly caused by the inductive effect of the phenyl substituents that leads to destabilization of the donor MO. (Funded by the DFG research unit 557 and the university of Bonn)

CPP 9.12 Mon 16:45 Poster A

Understanding Molecular Transport — ●ANGELICA ZACARIAS and EBERHARD K.U. GROSS — Institut für Theoretische Physik, Freie Universität Berlin, Germany

In the past, computers have grown increasingly powerful as their basic elements became smaller. Present-day silicon technology allows integrated circuits on the micron scale. With the advent of the new generation of High-k transistors the gate length reach sizes between 85-45nm. However to further reduce the size, device designs have to be replaced by new concepts which make use of the quantum mechanical effects that dominate the atomic scale. The basic idea of molecular electronics is to use single-molecules as the basic elements of the electronic devices. The flexibility of such "molecular transistors" originates in the sensitivity of the IV-characteristics to the subtle details of the molecules. Theoretical simulations of such systems can play a key role in unveiling the mechanisms that control molecular transport. Calculations have so far shown that the shape of IV characteristics is determined primarily by the electronic states of the molecule, as they evolve as a function of an applied bias, whereas the overall magnitude of the current is controlled by the details of the molecule-electrode contacts. Using a combined density-functional theory (DFT) and Green's function approach we present the IV-characteristics of C_{60} sandwiched between two gold metallic tips. Among other results we will present an encouraging comparison with experimental results of the conductance properties of C_{60} on Au(111).

CPP 9.13 Mon 16:45 Poster A

Nanopatterning of functional protein arrays — ●MARK SCHNIETZ¹, HELGE GROSSMANN², HARUN SOLAK³, ROBERT TAMPÉ², ANDREY TURCHANIN¹, and ARMIN GÖLZHÄUSER¹ — ¹Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld — ²Institute of Biochemistry, Biocenter, Johann Wolfgang Goethe-University, D-60438 Frankfurt — ³Laboratory for Micro and Nanostructuring, Paul Scherrer Institut, CH-5232 Villigen PSI

The ability to anchor oriented and functional protein arrays at the nanoscale affords useful materials for both fundamental research in biophysics/-chemistry and biotechnological and tissue engineering applications. In this contribution we present a novel approach to the fabrication of protein nanoarrays based on the combination of extreme UV interference lithography (EUV-IL) of self-assembled monolayers for the generation of chemical nanopatterns [1] (top-down) and biochemical tweezers, multivalent surface chelators [2] (tris-nitrilotriacetic acid, tris-NTA), for high affinity capturing of His-tagged proteins (bottom-

up). The functionality of the generated protein arrays was demonstrated under physiological conditions via specific, homogeneous, oriented and reversible immobilization of His6-tagged 20S proteasome and fluorescence labeled His10-tagged maltose-binding proteins [3]. Various highly periodic dot and line patterns with areas up to ~ 10 mm² and features from 1000 nm to 50 nm were built in this way. [1] A. Turchanin et al., *Small* 2007. [2] A. Tinazli et al., *Chem. Eur. J.* 2005, 11, 5249. [3] A. Turchanin et al., *Adv. Mater.* 2007.

CPP 9.14 Mon 16:45 Poster A

Linear and nonlinear mechanics of bundles of semiflexible filaments — ●FELIX SCHUELLER¹, CLAUS HEUSSINGER^{1,2}, and ERWIN FREY¹ — ¹Ludwig-Maximilians-Universität München, München, Germany — ²Université de Lyon I, LPMC, Villeurbanne, France

Bundles formed from semiflexible polymers play an important role in many physiological processes inside and outside of the cell.

We have previously defined a simple model ("wormlike bundle", WLB [1]) that describes the dynamical and statistical mechanical properties of semiflexible polymer bundles in terms of a mode-number dependent bending stiffness $\kappa(q)$.

While this treatment was restricted to in plane deformations of the bundle, we show here, how the WLB can be extended to a fully three-dimensional model that, in particular, includes twist deformations.

In this framework, we examine buckling instabilities under external force or torque. We solve the eigenvalue problem for determining the critical load as well as integrate numerically the nonlinear Euler-Lagrange equations to find the post-buckling bundle shapes.

[1] C. Heussinger, M. Bathe, and E. Frey, *Phys. Rev. Lett.* 99, 048101 (2007)

CPP 9.15 Mon 16:45 Poster A

High energy reflectivity studies of protein adsorption on functionalized surfaces — ●KAVEH SHOKUIE¹, MICHAEL PAULUS¹, FLORIAN EVERS¹, FEDERICA VENTURINI², SEBASTIAN SCHOEDER², and METIN TOLAN¹ — ¹Experimentelle Physik Ia/ DELTA, Technische Universität Dortmund, Maria-Goeppert-Meyer Str. 2, 44221 Dortmund — ²European Synchrotron Radiation Facility, Grenoble, France

Adsorption of several proteins (Lysozyme, Hemoglobin, α -lactalbumin) on functionalized surfaces was investigated using high energy X-ray reflectivity. The main interest is the effect of different substrate surfaces on the protein adsorption behaviour (e.g. conformational changes of the protein). The applied technique, X-ray reflectivity, makes it possible to determine the sample's density profile perpendicular to its surface with Angstrom resolution. The high energy reflectivities were taken at the ID15 beamline of the ESRF using 72.5 keV radiation. The high photon energy allows the in situ investigation of the protein adsorption at the solid-liquid interface.

CPP 9.16 Mon 16:45 Poster A

Biofilm adsorption on tailored substrates: Ellipsometry, AFM, SPR and neutron scattering results — ●HENDRIK HÄHL, HUBERT MANTZ, YVONNE SCHMITT, and KARIN JACOBS — Saarland University, Experimental Physics, D-66123 Saarbrücken, Germany

Whenever a protein solution is in contact with a material, the proteins will adsorb onto the surface. Everyday examples for this process are biofilms on teeth. This study aims to reveal the influence of surface properties on the adsorption process. Our results show that the adsorption kinetics of e.g. α -amylase is sensitive to the thickness of the oxide layer on top of the Si wafer. This is astonishing since the chemistry of the offered surfaces is identical, meaning that the short-range forces are not varied. Only the long-range forces are altered by a variation of the oxide layer thickness, and they play a central role for the adsorption kinetics. Theoretical models and simulations suggest that a variation of long-range forces can lead to conformational changes of the proteins during the adsorption. To test this hypothesis, experiments with atomic force microscopy (AFM), surface plasmon resonance (SPR) spectroscopy and ellipsometry as well as neutron reflectivity measurements have been performed.

CPP 9.17 Mon 16:45 Poster A

Nonlinear rheology of a glassy solution of semiflexible polymers — ●CHRISTIAN HUBERT¹, JENS GLASER¹, and KLAUS KROY^{1,2} — ¹ITP, Universität Leipzig, PF 100920, 04009 Leipzig — ²HMI, Glienicke Str. 100, 14109 Berlin

Recent experimental studies on purified solutions of the semiflexible biopolymer F-actin show a pronounced transition of shear softening

to shear stiffening behavior as a function of different physiological parameters. The results suggest a surprising invariance of the rheology of the F-actin solution with respect to the choice of the control parameter. This property is successfully explained by the recently introduced glassy wormlike chain (GWLC) model, where the nonlinear response is traced back to a strong stretching of the relaxation spectrum of an ordinary wormlike chain. The model incorporates two stretching parameters corresponding to the height of free energy barriers due to stickiness and steric (free volume) interactions respectively, slowing down the relaxation of the polymer. A comprehensive overview of the dependence of the stretching parameters and the shear modulus on the physiological parameters is given.

[1] Semmrich, Storz, Glaser, Merkel, Bausch, Kroy, PNAS, In Press (2007)

[2] arXiv: 0705.0490, arXiv: 0711.2427

CPP 9.18 Mon 16:45 Poster A

AFM Studies of Langmuir-Blodgett Films of Acidic Peptides — ●MANUELA PLUNTKE¹, HAOFEI GONG², YI YANG³, NORBERT SEWALD³, DIRK VOLKMER², and OTHMAR MARTI¹ — ¹Institute of Experimental Physics, Ulm University, D-89069 Ulm — ²Institute of Inorganic Chemistry II, Ulm University, D-89069 Ulm — ³Faculty of Chemistry (AC 1), University of Bielefeld, PO Box 100 131, 33501 Bielefeld

Acidic proteins are found to play an important role in biomineralization. Extracted from different calcified tissues, they were shown to control polymorph selection, texture and morphology of CaCO₃ crystals. We recently fabricated Langmuir-Blodgett Monolayers of different artificial acidic peptides with β -hairpin conformation (H-Asp-(Phe-Asp)₃-D-Pro-Gly-Asp-(Phe-Asp)₃OH, H-Glu-(Phe-Glu)₃-D-Pro-Gly-Glu-(Phe-Glu)₃OH). Circular Dichroism Spectra show that these two peptides take a random coil and β -sheet structure in HFIP solution, respectively. At the air/water interface, significant differences of the peptide monolayer properties were found as revealed by surface pressure-area isotherms and BAM, although they have similar primary structure. Moreover, crystallization of CaCO₃ beneath these monolayers revealed different crystal morphologies. For a more detailed analysis of the peptide arrangement at interfaces we transferred the monolayers on mica and investigated them by means of high resolution AFM. Based on preliminary studies we assume that only the peptide H-Glu-(Phe-Glu)₃-D-Pro-Gly-Glu-(Phe-Glu)₃OH forms a highly ordered lattice of hairpin structures.

CPP 9.19 Mon 16:45 Poster A

Carbon dioxide hydrate formation at the carbon dioxide - water interface — ●FELIX LEHMKÜHLER¹, MICHAEL PAULUS¹, CHRISTIAN STERNEMANN¹, DANIELA LIETZ¹, FEDERICA VENTURINI², and METIN TOLAN¹ — ¹Technische Universität Dortmund, Experimentelle Physik I/DELTA, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany — ²ESRF, BP 220, 38043 Grenoble Cedex 9, France

The formation of gas hydrate at the water - carbon dioxide interface was studied by x-ray reflectivity and x-ray diffraction experiments. CO₂ forms under high pressures and low temperatures cubic water cages with a lattice constant of 12 Å (structure I hydrate) and a CO₂ molecule in the center. At a temperature of 0°C a minimum pressure of 12.5 bar is required for CO₂ hydrate stability. In nature this formation takes usually place at the water - gas interface due to a higher gas concentration in comparison with the water bulk. However, the microscopic formation process is still not understood.

The water - CO₂ interface was investigated at a temperature of 0°C and gas pressures up to the condensation pressure of CO₂ of 35 bar. A pressure dependent adsorption of thin CO₂ layers is observable, but no hydrate formation. In contrast, after rising the gas pressure to condensate a macroscopic thick CO₂ layer hydrate crystallites could be observed at the liquid-liquid interface using x-ray diffraction.

To investigate this formation more precisely diffraction patterns were measured at different height positions of the sample. Hydrate clusters were observable at all positions except the gas phase. However, the highest formation rate is found at the water - liquid CO₂ interface.

CPP 9.20 Mon 16:45 Poster A

Lysozyme Adsorption at the Silica/Water Interface: an in situ High Energy X-ray Reflectivity Study — ●FLORIAN EVERS, KAVEH SHOKUIE, MICHAEL PAULUS, CHRISTIAN STERNEMANN, and METIN TOLAN — TU Dortmund, Fakultät Physik/DELTA, Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany

Lysozyme adsorption at the silica/water interface has been studied us-

ing high energy x-ray reflectivity which is a well-established method to study the structure of thin films. Data on protein layers adsorbed at solid/liquid interfaces are still rare. The dispersion profile of adsorbed lysozyme layers at hydrophilic silica interfaces, the effect of pH and protein concentration of the aqueous solution on the adsorption, and the time-dependence of the adsorption process were studied. Our observation of lysozyme monolayer adsorption is partially in contrast to former measurements with neutrons and to predictions.

CPP 9.21 Mon 16:45 Poster A

The Effect of electrolytes on interactions in thin aqueous wetting films — ●NATASCHA SCHELERO, KATARZYNA HÄNNI-CIUNEL, and REGINE VON KLITZING — Stranski-Laboratorium, Institut der Chemie, TU Berlin, Strasse des 17. Juni 124, D-10623 Berlin

The (de)stability and functionality of thin wetting films plays an important role for processes in technical applications. The forces between the opposing interfaces depend on the composition of the film interfaces and of the film fluid. In the present paper the sum of interactions between the film surfaces is determined quantitatively by the disjoining pressure isotherm and it is measured by varying the outer pressure in a thin film pressure balance. Usually, this apparatus is used for disjoining pressure measurements at free-standing foam films (air/liquid/air). In recent studies we showed that it also can be used for the investigation of wetting films (air/liquid/solid) [1]. Water films in presence of 0.1 mM NaCl are stable against negatively charged interfaces like bare Silicon or Silicon coated with negatively charged polyelectrolytes, but unstable against positively charged surfaces. The films become thinner and less stable with increasing ionic strength indicating that the forces within the water film are controlled by electrostatic interactions [2]. The results give a clear evidence for negative charges at the free air/water interface [3]. Further on, the effect of specific ions on the stabilisation by electrostatic interfacial repulsion is investigated. [1] R. v. Klitzing, *Adv. Coll. Interf. Sci.*, 2005,114/115:253 [2] Hänni-Ciunel K. et al., *Soft Materials*, 2007, 5 (2), 61-73 [3] Ciunel K. et al., *Langmuir* 2005 21 4790 - 4793

CPP 9.22 Mon 16:45 Poster A

Investigations on the Structure and Dynamics of DMPC-Monolayers used as Stabilizers in Colloidal Dispersions — ●SEBASTIAN BUSCH, CHRISTOPH SMUDA, and TOBIAS UNRUH — Forschungsneutronenquelle Heinz Maier-Leibnitz and Physik Department E13, Technische Universität München, Munich, Germany

Many modern drugs are not water-soluble. To facilitate their intravenous applicability, a drug carrier has to be employed. Dispersions of lipid nanoparticles stabilized by dimyristoylphosphatidylcholine (DMPC) are promising candidates. It has been shown [1] that not only the drug release rate but also the storage stability of these systems highly depends on the properties of the stabilizer. These properties were investigated i. a. by small angle X-ray scattering [2], revealing that the structure of the monolayer is clearly distinct from the well-known structure of bilayers. A series of experiments aiming to determine the dynamic characteristics of DMPC-monolayers was carried out at the cold neutron time-of-flight spectrometer TOFTOF at the Forschungsneutronenquelle Heinz Maier-Leibnitz in Garching bei München. First results are presented and discussed.

[1] K. Westesen, B. Siekmann, *Int. J. Pharm.*, 151 (1997) 35; H. Bunjes, M. H. J. Koch, K. Westesen, *J. Pharm. Sci.* 92 (2003) 1509; H. Bunjes, F. Steiniger, W. Richter, *Langmuir* 23 (2007) 4005

[2] T. Unruh, *J. Appl. Cryst.* 40 (2007) 1008

CPP 9.23 Mon 16:45 Poster A

Microscopic theory of liquid-vapour interface of simple fluids — ●VITALIE BOTAN and MARTIN OETTEL — Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, Mainz, Germany

The liquid-vapor interface of Lennard-Jones fluids is examined by combining integral equation and density functional theory. In this approach a closure of reference hypernetted chain type to the inhomogeneous Ornstein-Zernike equation for the correlations functions is developed employing a bridge functional (instead of a bridge function) of a suitably chosen hard-sphere reference system. Using Tarazona's free energy functional for the reference system, the obtained self-consistent solutions for the density profiles and inhomogeneous two-body correlation functions are analyzed with respect to the mesoscopic capillary wave picture.

CPP 9.24 Mon 16:45 Poster A

Temperature dependent (2D) ordering in monolayers of amphiphile molecules — ●SASKIA SCHMACKE¹, BERND STRUTH², LUTZ WIEGART³, HENRI GLEYZOLLE³, MICHAEL PAULUS¹, and METIN TOLAN¹ — ¹Fakultät Physik /DELTA, Technische Universität Dortmund, D-44221 Dortmund, Deutschland — ²DESY, D-22602 Hamburg, Deutschland — ³ESRF, B.P. 220, 38043 Grenoble Cedex, France

Layers of amphiphile molecules on liquid substrates show a different phase behaviour depending on environmental parameters such as temperature, surface pressure and subphase. In this work the solid phase of the Phospholipid monolayer DPPC (dipalmitoyl-glycerophosphocholine) was analysed in order to investigate the influence of temperature on the crystalline structure of the layer. The latter was determined by the use of the Grating Incidence X-Ray Diffraction technique (GID) at the beamline ID10b, ESRF. The obtained diffraction spectra are analysed in two steps: First the information about the 2D unit cell of the crystalline phase, e.g. lattice spacings, lattice type (2D Bravais lattice) and the deformation of the lattice was determined. In the second step the intensity dependence on the wave vector transfers perpendicular to the surface was analysed leading to information about the scatterer itself. Thus, chain length, diameter, tilt angle and orientation within the lattice of the molecules forming the monolayer are determined. A temperature induced phase transition from a centred rectangular to a hexagonal lattice with decreasing temperature was observed.

CPP 9.25 Mon 16:45 Poster A

Estimation of spinodals in pure fluids from interfacial properties obtained from equilibrium molecular dynamics and lattice Boltzmann simulations — ATTILA IMRE¹, GUSZTAV MAYER¹, GABOR HÁZI¹, ROBERTO ROZAS^{2,3}, and ●THOMAS KRASKA³ — ¹Simulator Development Department, KFKI Atomic Energy Research Institute — ²Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, D-51147 Köln — ³Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln

In this work, local pressure and density profiles of a liquid film in contact with its vapor at equilibrium are calculated. Two methods are employed; molecular dynamics and lattice Boltzmann simulations. The set of local values of tangential pressure and density along a liquid-vapor interface exhibits a van der Waals-like loop. The loci of the extreme values of local tangential pressure in the interfacial profile are related to the spinodal state. The maximum and minimum values of the tangential pressure are linearly related to the vapor and liquid spinodal pressures, respectively. The coefficient of the relationship appears to be universal and of geometrical origin. Comparison of the spinodal curves obtained from equations of state shows good agreement with the simulation results. Based on this investigation a method is proposed for the estimation of the liquid spinodal from experimental data. Estimations for water and helium are presented.

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Heterogeneous nucleation and growth of high wetttable systems studied by molecular dynamics simulations — ●ROBERTO ROZAS^{1,2} and THOMAS KRASKA² — ¹Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt, Linder Höhe, D-51147 Köln — ²Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, D-50939 Köln

Heterogeneous nucleation and growth of supersaturated argon vapor at polyethylene surfaces is investigated by molecular dynamics simulations. The system serves as a model for high wetttable systems. A non-equilibrium ensemble which allows the development of gradients in the system is employed; Nosé-Hoover thermostat is applied to the polymer substrate only while the vapor condenses. Simulations along an isotherm at different initial saturation of the vapor indicate a transition, close to the binodal, from adsorption to heterogeneous nucleation. At moderate saturation the layer-by-layer growth mechanism dominates while at higher supersaturation a tendency to growth islands-on-layers growth is observed. We find for this system that a two-dimensional version of the classical heterogeneous nucleation theory (HEN2D) is most suitable to describe the nucleation rate data versus saturation obtained from simulation.