CPP 15: P1: Interfaces and Thin Films

Time: Monday 16:00–19:00 Location: Poster A

CPP 15.1 Mon 16:00 Poster A

Study of contraction/spreading of microdroplets — •Tak Shing Chan[1,2], Joshua D. McGraw[1], Simon Maurer[1], Thomas Salez[3], Michael Benzaquen[3], Elie Raphaël[3], Karin Jacobs[1], and Martin Brinkmann[1,2] — [1]Saarland University, Saarbrücken, Germany — [2]Max-Planck institute, Göttingen, Geermany — [3]ESPCI, Paris, France

A non-equilibrium liquid drop sitting on a smooth substrate will contract or spread depending on the microscopic contact angle and the initial shape of the drop. Previous studies assume a huge separation of length scales between the drop size R and the slip length b, as a result the drop remains as a spherical cap and interface deformations due to viscous effects are localized in a small region near the contact line . A well-known example is a drop spreading over a completely wetting surface, which follows Tanner*s law. In this project, we both experimentally and theoretically investigate contraction/ spreading of micro-droplets in the regimes where these two length scales are not far separated. Instead of a quasi-static shape during the evolution, the profiles display more structures in these regimes.

CPP 15.2 Mon 16:00 Poster A

Investigations on ZnO scattering layers for OLED applications — •Lorenz Biessmann, Christoph J. Schaffer, Johannes Schlipf, Volker Körstgens, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85738 Garching

By now the internal quantum efficiency of organic light-emitting diodes (OLEDs) reached values close to 1 but the overall efficiency still suffers on the extraction of the photons from the device. For further improvements of the performance one can apply a scattering layer to the device. Besides the direct structuring of the substrate surface, the attachment of a transparent layer on the substrate is a very promising approach. With an optical band gap of 3.3 eV, ZnO is a suitable material for this method. In this work ZnO is used as an additional layer on a glass substrate to achieve scattering abilities. For this purpose a structure giving diblock copolymer template was combined with sol-gel chemistry for tailoring the ZnO scattering layer. This yields thin films with nano- and micro-structures. The film morphology as probed by scattering techniques and SEM is related to the spectral response to gain a structure-function relationship.

CPP 15.3 Mon 16:00 Poster A

Monte Carlo Simulation of Thin Film Polymer Melts — •Andre Galuschko[1], Michael Lang[1], Torsten Kreer[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Hohe Straße 6, 01069 Dresden, Germany. — [2]Institute of Theoretical Physics, Technische Universität Dresden, Zellescher Weg 17, 01062 Dresden, Germany.

We present Monte Carlo simulation data on conformations and dynamics of polymer melts confined in narrow slits of different widths and compare with data of bulk systems. We find that in confined geometries the chains swell laterally, they retain and even expand their spatially long-range correlations as compared to bulk polymers and in contrast to the assumption of a complete screening of excluded volume. Long chains in bulk melts show entangled dynamics with a clear signature of a $t^{1/4}$-power law for the mean square displacements of innermost monomers at intermediate time scales. This behavior is gradually lost by confining the melts in slits with decreasing width. For ultra-thin films, the dynamics appears to follow a $t^{1/2}$ dependence over the entire sub-diffusive regime. However, the terminal relaxation time is significantly increased as compared to Rouse relaxation. This interesting observation was not reported previously and is the focus of our ongoing research.

CPP 15.4 Mon 16:00 Poster A

Molecular dynamics simulation of the interaction of polyamines with silica substrates — •Sergii Donets, Arezoo Dianat, Rafael Gutierrez, Manfred Bobeth, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany

The role played by organic components in the process of biosilification, resulting in well-defined three-dimensional silica structures in algae, has not been completely clarified. Especially in the case of diatoms several organic components have been meanwhile identified, including silaffins, silacidins, and polyamines. In this study we perform classical and quantum molecular dynamics simulations addressing two major issues related to polyamines: 1) the possible protonation states and protonation sites in short polyamines, and 2) the interaction of differently protonated polyamines with silica surfaces in order to identify the possible molecular conformations in dependence on the degree of protonation. Our results are in good quantitative agreement with results based on NMR experiments.

CPP 15.5 Mon 16:00 Poster A

Structural investigation of ferrocene containing polymers in thin films and at the liquid/air interface — •Haiko Didzoleit[1], Markus Gallei[2], Johannes Elbert[2], Matthias Rehahn[2], and Bernd Stühn[1] — [1]TU Darmstadt, Experimental Condensed Matter Physics — [2]TU Darmstadt. Ernst-Berl-Institut für Technische und Makromolekulare Chemie

We focus on amphiphilic ferrocene block copolymers (here poly(vinyl ferrocene)-b-poly(vinyl pyridin), PVFc-P2VP and poly(ferrocenylsilane)- poly(vinyl pyridin) PFS-P2VP) and their structural properties at liquid/air and solid/air interfaces. These films are prepared as Langmuir monolayers on a water substrate and as Langmuir-Blodgett multilayer films on a solid silicon substrate. The structural properties are monitored by X-Ray reflectivity in situ (water subphase) and ex situ (silicon substrate) and analysed in terms of standard models.

The structure of the Langmuir monolayer is dominated by the P2VP block partner and strongly ruled by the surface pressure in the monolayer. Besides their structural changes the ferrocene moiety can be reversibly switched from diamagnetic to paramagnetic state by oxidation/reduction. We determine the magnetic properties of thin films by SQUID magnetometry. The oxidised state induces a conformational change leading to a swelling of the polymer film on solid substrates and to increasing solubility in water. The impact of these external variables on the structural properties will be shown for different composites of the diblock copolymer.

CPP 15.6 Mon 16:00 Poster A

Simultaneous Mapping of Long-Range Attractive Forces and Near-Surface Interaction Forces with Multi-Set point Intermittent Contact (MUSIC) Mode AFM — •Diana Voigt, Eike-Christian Spitzner, and Robert Magerle — Technische Universität Chemnitz, Chemnitz, Germany

Studies using intermittent contact (IC) mode atomic force microscopy (AFM) often focus on imaging the surface morphology and on understanding contrast formation due to the mechanical response of the specimen. Here we study the contribution of long-range interactions, such as electrostatic and van der Waals interactions, as well as local differences in hydrophobicity using MUSIC mode AFM. Substrates partially covered with self-assembled monolayers either with carbon or amine terminated tail groups are studied. This mimics protein surfaces with locally different degrees of hydrophobicity. We aim at a detailed understanding of long-range and near-surface tip-sample interactions under different conditions. A methodological point of interest is the question about the ability to measure the different interactions in one single-pass measurement using MUSIC mode AFM.

CPP 15.7 Mon 16:00 Poster A

Accurate Refractive-Index Determination from First- and Second-Order Critical Angles of Periodic Surface Patterns — •Christoph Meichner[1], Lothar Kador[1], Andreas Schedl[2], Hans-Werner Schmidt[2], Christian Neuber[2], and Klaus Kreger[2] — [1]University of Bayreuth, Institute of Physics and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany — [2]University of Bayreuth, Macromolecular Chemistry I and Bayreuth Institute of Macromolecular Research (BIMF), 95440 Bayreuth, Germany

We present a novel method for the determination of the refractive-index dispersion of transparent solid films. The approach is based on irradiating collimated monochromatic light onto the sample with the il-

luminated spot carrying a periodic surface pattern. A simple rotational stage is sufficient for measuring critical angles of the light propagating in the film. From these angles, the refractive indices are calculated. To study the accuracy of our method, we prepared samples of a PDMS cast resin (*Sylgard*® 184) and compared the results to those obtained with an Abbe refractometer. The data are in good agreement, considering the angular resolution of the stage and the precision of the grating constant.

CPP 15.8 Mon 16:00 Poster A

Ultrafast structural dynamics of membrane-bound water molecules revealed by two-dimensional surface-specific vibrational spectroscopy — •Ruth Livingstone[1], Zhen Zhang[1], Lukasz Piatkowski[2], Huib J. Bakker[2], Mischa Bonn[1], and Ellen H. G. Backus[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

We explore the structure and structural dynamics of water in contact with a model lipid membrane (a DPTAP monolayer) using ultrafast time-resolved 2-dimensional sum-frequency generation spectroscopy. With this highly surface-specific technique we monitor the ultrafast frequency fluctuations of the O-H stretch vibrations, that directly reflect the structural dynamics of the water hydrogen-bonding network. For water interacting with a lipid membrane the frequency correlations decay on a sub-picosecond timescale. This timescale does not change upon isotopic dilution of the water, revealing that the fast spectral dynamics are not the result of Förster energy transfer, as previously observed at the water-air interface, but rather result from ultrafast fluctuations in the local hydrogen-bonding network of membrane-bound water molecules.

CPP 15.9 Mon 16:00 Poster A

Optical Tracking of Single Ag Clusters in Nanostructured Water Films — •Stefan Krause, Martin Hartmann, Ingolf Kahle, Martin Neumann, Mario Heidernätsch, Stefan Spange, and Christian von Borczyskowski — Technische Universität Chemnitz

Beside organic fluorescent molecules inorganic nano particles have attracted increasing attention as optical probes for soft matter during the past two decades. Especially the photo stability of inorganic materials makes them suitable as fluorescent labels and nano probes. Thereby the fluorescence of a single particle serves as a sensitive probe for its environment and changes of the fluorescence lifetime, emission wavelength, polarization and position can report spatial and temporal heterogeneities in the environment of the particles which are not accessible with ensemble methods. Here we report on the spatial diffusion of single silver nano clusters of the size of about one nano meter within structured water layers on pure SiO2. The diffusion reveals a twofold spatial heterogeneity of the water films. The interaction of water molecules with the surface results in an *ice-like* structuring of the first 2 to 3 mono layers while higher layers exhibit an unstructured, *water-like* formation of the molecules. In addition, irregularities in the density of surface silanols which can be influenced by different surface treatment processes leads to formation of lateral islands. As a result of this structuring diffusion shows immobile, slow and fast diffusing clusters. This experiment provides insights into the processes of water film formation and its heterogeneities.

CPP 15.10 Mon 16:00 Poster A

Interfacial melting of ice confined in layered sheet silicates — •Hailong Li[1], Julian Mars[1], Johannes Grosse[1], Thomas Buslaps[2], and Markus Mezger[3,1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Johannes Gutenberg-Universität Mainz, Germany

Most of the fresh water on earth is stored in the form of ice. Ground ice and permafrost contain 3 times more fresh water than all the lakes. The material properties of these permafrost composites strongly depend on the molecular scale structure of the ice/solid interface. Early in 1859, Faraday proposed the existence of a liquid-like layer at ice surfaces. Interfacial melting at well-defined single crystalline ice/solid interfaces was studied by x-ray reflectivity and other techniques. However, the understanding of the interfacial melting of ice and the structure of the liquid-like layer is still under debate. Layered sheet silicates such as exfoliated vermiculite are ideal materials to study the interfacial melting of ice in a geologically relevant system. We employ high-energy x-ray diffraction to measure the temperature dependence of the crystalline ice fraction in ice/vermiculite composites with a high interface to volume ratio. From the anisotropy of the ice reflections in textured samples with aligned vermiculite sheets we extract the preferred orientation of the confined ice crystals.

CPP 15.11 Mon 16:00 Poster A

Influence of adhesion on composite mechanical and electric properties of thin Poly(3-hexylthiophene-2,5-diyl) (P3HT) films on stiff substrate (ITO electrode on glass) by means of AFM Force Distance Curves (FDC) and conductive AFM — •Dorothee Silbernagl[1], Christiane Weimann[1], and Heinz Sturm[1,2] — [1]BAM Federal Institute for Materials Research, Berlin, Germany — [2]Technical University Berlin IWF, Berlin, Germany

Mechanical properties of thin polymer films on stiff substrates have been investigated by AFM FDC and are known to be a composite of the properties of both materials. The contribution of each material to the resulting module depends primarily on film thickness. Films act as mechanical "insulator" with regard to the substrate[Si1]. The additional influence of adhesion between film and substrate has been demonstrated: the higher adhesion the better mechanical properties are "conducted", increasing the influence of substrate's mechanical properties on composite module[Si2]. We propose an analogy between the mechanical conductivity and the electric conductivity which can be exploited to quantify the influence of the adhesion. Conductive polymer films (P3HT) on a substrate/electrode (glass/ITO) have been measured using AFM FDC and conductive AFM. For this purpose spin coated films of P3HT (30nm<t<150nm)on ITO substrates have been aged to induce partial delamination. Film properties and their changes due to aging have been monitored by confocal Raman spectroscopy. [Si1] Silbernagl, Cappella. Surface Science, 2009, 603(16),2363-2369. [Si2] Silbernagl, Sturm, Cappella. Langmuir, 2009, 25(9),5091-5097.

CPP 15.12 Mon 16:00 Poster A

Shape and Wrinkle Analysis of deflated Elastic Capsules — •Jonas Hegemann, Sebastian Knoche, and Jan Kierfeld — TU Dortmund, 44221 Dortmund, Germany

Elastic capsules, prepared from droplets or bubbles attached to a capillary (as in a pendant drop tensiometer), can be deflated by suction through the capillary. We study this deflation and show that a combined analysis of the shape and wrinkling characteristics enables us to determine the elastic properties in situ. Shape contours are analyzed and fitted using shape equations derived from nonlinear membrane-shell theory to give the elastic modulus, Poisson ratio and stress distribution of the membrane. We include wrinkles, which generically form upon deflation, within the shape analysis. Measuring the wavelength of wrinkles and using the calculated stress distribution gives the bending stiffness of the membrane. We compare this method with previous approaches using the Laplace-Young equation and illustrate the method on polymerized octadecyltrichlorosilane (OTS) capsules. Our results are in agreement with the available rheological data.

CPP 15.13 Mon 16:00 Poster A

Influence of the chemical structure on the slip boundary condition of liquids — •Mischa Klos[1], Sebastian Backes[1], Juan Manuel Castillo Sanchez[2], Hans Hasse[2], and Karin Jacobs[2] — [1]Saarland University, Experimental Physics, D-66123 Saarbrücken — [2]TU Kaiserslautern, Laboratory of Engineering Thermodynamics, D-67663 Kaiserslautern

On small scales, especially in microfluidic devices, the role of the solid/liquid interface gets more important for the flow dynamics. Our experiments probe slippage via the dewetting of thin polymer films on hydrophobic substrates [1]. As hydrophobic coatings we use amorphous polymers (AF1600, AF2400) and different types of highly ordered self-assembled silane monolayers on top of silicon substrates. On silane surfaces, polystyrene (PS) of low molecular weight exhibit slip lengths up to micrometers [2]. On AF1600, no significant slip is observed . Scattering studies reveal an ordering of the PS side chains at the solid/liquid interface depending on the structure of the substrate [3]. Recent simulations were able to characterize the used SAMs[4]. However, the situation changes if PMMA or polyvinylpyridine (PVP) are used: Dewetting experiments show that slip is less pronounced in PVP and in PMMA films. Obviously, the structure of the side groups play a significant role. X-ray reflectometry supplement this hypothesis and give further insight to the slippage mechanism at the solid/liquid interface. [1] O. Bäumchen, et.al., J Phys Condens Mat 24 (2012) 325102 [2] R. Fetzer, et. al, Europhys Lett 75 (2006) 638 [3] P. Gutfreund, et. al.,Phys Rev E 87 (2013) 012306 [4] J.M. Sanchez, et. al.

submitted

CPP 15.14 Mon 16:00 Poster A

Molecular scale structures of ionic liquid interfaces under electric potential — •Julian Mars[1], Peter Reichert[1], Kasper Skov Kjaer[2], Tim Brandt van Driel[2], Martin Meedom Nielsen[2], Moshe Deutsch[3], and Markus Mezger[1,4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Centre for Molecular Movies, Department of Physics, TechnicalUniversity of Denmark, Lyngby, Denmark — [3]Department of Physics and Institute of Nanotechnology andAdvanced Materials, Bar-Ilan University, Ramat-Gan, Israel — [4]Johannes Gutenberg-Universität Mainz, Germany

Electrolyte interfaces under electric potential are of a great scientific and technological interest. For diluted electrolyte solutions, the interfacial ion profile can be described by the Gouy-Chapman theory. However, for solvent-less electrolytes such as ionic liquids the diluted solution approximation is clearly invalid. Despite of their importance, the molecular scale structure of ionic liquids near electrodes is still under debate. We have studied the potential dependent interfacial structure of room temperature ionic liquids with high-energy x-ray reflectivity and impedance spectroscopy measurements. We find oscillatory charge density profiles consisting of alternating anion- and cation-enriched layers at both cathodic and anodic potentials. This structure is shown to arise from the same ion-ion correlations dominating the liquid bulk structure. The relaxation dynamics of the interfacial structure were studied by impedance spectroscopy and time resolved x-ray reflectivity experiments with sub-millisecond resolution.

CPP 15.15 Mon 16:00 Poster A

Alginate - Chitosan Multilayer Films and Their Properties — •Hakan Kaygusuz[1,2], F. Bedia Erim[2], and Regine von Klitzing[1] — [1]Stranski-Laboratorium für Physikalische und Theoretische Chemie, Technische Universität Berlin, Strasse des 17. Juni 124, D-10623 Berlin, Germany — [2]Department of Chemistry, Istanbul Technical University, 34469 Maslak, Istanbul, Turkey

Alginate and chitosan are oppositely charged polysaccharides, being anionic and cationic, respectively. These polysaccharides have many uses, both crosslinked and uncrosslinked. Negatively charged surfactant, sodium dodecyl sulfate (SDS), has effects on viscosity and mechanical properties of linear and crosslinked alginate structures. For example addition of SDS decreases the viscosity of the alginate solutions and increases the Young's modulus of crosslinked alginate gels. Therefore it is aimed to observe the ability of forming multilayer films with these materials and the effect of SDS on the film structure.

Multilayers of these polyelectrolytes were prepared using dip-coating method. The properties such as film thickness and roughness were characterized using ellipsometry, atomic force microscopy and X-ray reflectometry. The effect of sodium chloride and sodium dodecyl sulfate concentration, and the number of double layers on film properties were observed. The crosslinking and swelling ability of these films were discussed.