CPP 19: Poster: Interfaces and Thin Films

Time: Tuesday 18:00–20:00 Location: P2

CPP 19.1 Tue 18:00 P2

Kinetics of structural changes in lamellar poly(styrene-b-butadiene) diblock copolymer thin films during thermal treatment — •Alessandro Sepe[1], Dorthe Posselt[2], Sebastian Jaksch[1], Eicke Tilo Hoppe[1], David Magerl[1], Qi Zhong[1], Jan Perlich[4], Detlef-Matthias Smilgies[3], and Christine M. Papadakis[1] — [1]TU München, Physikdepartment, Physik der weichen Materie, Garching, Germany — [2]Institute for Science, Systems and Models, Roskilde University, Denmark — [3]Cornell High-Energy Synchrotron Source (CHESS), Ithaca, U.S.A. — [4]HASYLAB at DESY, Hamburg

Nanostructured block copolymer thin films find a number of applications, especially for optical elements. Thermal annealing has frequently been applied to remove defects and to improve the long-range order. Annealing temperature is a key parameter because it influences both, the interfacial tension between the two blocks and the polymer mobility. We wish to elucidate the mechanisms of structural changes induced by thermal treatment. In-situ grazing-incidence small-angle X-ray scattering and VIS interferometry as well as ex-situ atomic force spectroscopy and X-ray reflectivity were used. The poly(styrene-b-butadiene) system studied by us is well-suited to address this question because it has initially the perpendicular lamellar orientation. We have found that for annealing temperatures below the glass transition temperature of the PS block and subsequent cooling to room temperature, the lateral order is improved, whereas above, a random lamellar orientation and subsequent destruction of structure is observed.

CPP 19.2 Tue 18:00 P2

Strong segregation limit of a diblock copolymer film in an electric field — •Michael Harrach, Barbara Drossel, Marianne Heckmann, and Tiago de Paula Peixoto — Institut für Festkörperphysik, TU Darmstadt

We present an algorithm to evaluate the free energy of a thin film of diblock copolymers in an electric field at low temperatures. We apply the strong-segregation limit, where only one type of monomer is present in each domain. We assign different dielectric constants to the two types of domains. We consider a two-dimensional system, assuming translational invariance in the third dimension, and periodic boundary conditions in the direction parallel to the condensator plates, between which the polymer film is confined. We evaluate the different contributions to the free energy for different types of phases, with the goal to find the phase with the lowest free energy as a function of the film thickness and the applied electric field.

CPP 19.3 Tue 18:00 P2

Control of Lamella Orientation in Confined Block Copolymer Films — •Vanessa Weith, Alexei Krekhov, and Walter Zimmermann — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth, Germany

The study of phase separation in polymer blends offers substantial opportunities to control the morphology of the evolving patterns. This is of considerable fundamental and technological importance in order to develop new materials to achieve specific properties. New strategies to control the long-range order in the nanostructures formed by microphase separation in block copolymers can be developed with the help of recently found thickness-dependent lamella orientation in diblock copolymer films [1].

We have studied this issue using a mean-field approach. Investigating the existence, stability and free energy of lamellar solutions in infinite and confined geometries in one spatial dimension, the results agree with those of other models based on self-consistent field theory [2] or free energy [3]. Extending the analysis to two spatial dimensions helps to determine which orientation of the lamella is selected depending on the input parameters. Furthermore the dynamics of the spatio-temporal behavior of the phase separation process is characterized.

[1] V. Olszowka, L. Tsarkova, and A. Böker, Soft Matter 5, 812 (2009)

[2] M. W. Matsen, J. Chem. Phys. 106, 7781 (1997)

[3] D. G. Walton, G. J. Kellog, and A. M. Mayes, Macromolecules 27, 6225 (1994)

CPP 19.4 Tue 18:00 P2

Calorimetric investigations of thin films of micelles formed by triblockcopolymers — •Heiko Huth[1], Julia Gensel[2], Andreas Fery[2], and Christoph Schick[1] — [1]Universität Rostock, Institut für Physik, Wismarsche Straße 43-45, 18051 Rostock, Germany — [2]Universität Bayreuth Physikalische Chemie II, Universitätsstraße 30, 95440 Bayreuth, Germany

In the recent years investigations in the nano sized range is in the focus of many researchers. For basic understanding as well as for practical applications the behavior of thin films and other confinements in small dimensions is of interest.

As one example for applications there is the idea of structured thin films due to self assembly i.e. of complex substructures as micelles. While for structural investigations several methods for thin films are present it is difficult to find methods to observe dynamic properties. AC-chip calorimetry has demonstrated the ability to measure thin polymeric films [1] and is now used as a very sensitive tool for calorimetric investigations of thin films formed by micelles.

[1] Huth, H., Minakov, A. A., Schick, C., J. Polym. Sci. B Polym. Phys. 2006 44: 2996.

CPP 19.5 Tue 18:00 P2

Structure formation and dynamics of thin liquid crystal (8CB) films depending on the type of substrate — Benjamin Schulz[1,2], •Daniela Täuber[1], and Christian von Borczyskowski[1] — [1]nanoMA, TU-Chemnitz, Institut für Physik — [2]now at MPI-DS, Göttingen

Taylor made single dye molecules were used to study structure and dynamics within 220 nm thick liquid crystal films. While the diffusion is strongly heterogeneous for thin 8CB films [1] on Si wafers with native SiOx as well as with 100 nm thermally grown SiOx, the structure of the film differs: On 100 nm SiOx, the liquid crystal self-organizes into focal conic domains [2], while on native SiOx a terraced structure with holes is observed. Using dye molecules which align with the liquid crystal, a correlation between structure and dynamics is shown.

[1] B. Schulz, D. Täuber, F. Friedriszik, H. Graaf, J. Schuster and C. von Borczyskowski: PCCP 12 (2010) 11555

[2] V. Designolle, S. Herminghaus, T. Pfohl, und Ch. Bahr: Langmuir 22 (2006) 363

CPP 19.6 Tue 18:00 P2

Equilibrium geometry of three smectic liquid crystalline films — •Torsten Trittel[1], Ruth Aldred[2], and Ralf Stannarius[1] — [1]Otto-von-Guericke Universität, Institut für experimentelle Physik, 39106 Magdeburg — [2]The University of Exeter, School of Physics, Exeter EX4 4QL

We spotlight the geometrical properties of Plateau borders in an arrangement of connected fluid free standing films. In our experiment, a circular Plateau border surrounds a planar smectic film and connects it with two smectic catenoids. We show that similar to soap films, the geometry can be described by a negative line tension of the circular contact region. It is obvious that the equilibrium angle between the films depends upon the liquid content in the contact region, and with increasing liquid content, deviations from Plateau's rule are observed. The results are qualitatively comparable to soap films. A possible origin of slight quantitative differences is discussed.

CPP 19.7 Tue 18:00 P2

Interactions and stability of foam films from oppositely charged surfactant mixtures — •Heiko Fauser, Nora Kristen-Hochrein, Natascha Schelero, and Regine von Klitzing — Stranski-Laboratorium, Institut für Chemie TU-Berlin, Strasse des 17. Juni 124, 10623 Berlin, Deutschland

Mixtures of cationic and anionic surfactants are widely used in industrial processes and products. Until this date mainly the adsorption behavior of oppositely charged surfactants at liquid and solid surfaces has been investigated. In order to understand adsorption at foam films it is important to investigate free-standing foam films. A measurement of the interactions between two opposing foam-film interfaces is the disjoining pressure, which is considered to be the sum of repulsive electrostatic and steric forces, as well as attractive van der Waals forces. The disjoining pressure is measured with a so called Thin Film

Pressure Balance.

Mixtures of oppositely charged surfactants tend to show interesting properties and behavior in terms of stability and thickness of the free-standing films. For example is the formation of a Common Black Film or a much thinner but more stable Newton Black Film governed by the concentration ratio of the surfactant mixture.

Also the question how supplement measurements of other physical properties like surface tension or surface rheology can support to understand our results and help to develop a more precise description of such surfactant mixtures is taken into account.

CPP 19.8 Tue 18:00 P2

Structures in molecular thin smectic liquid crystal films — •Benjamin Schulz and Christian Bahr — MPI for Dynamics and Self-Organization, Bunsenstraße 10, 37073 Göttingen

We present a convenient technique to create thin films of the smectic liquid crystal 8CB with a defined number of molecular layers on silicon surfaces. Using AFM- and ellipsometry-measurements we observe characteristic porous surface textures that are common to all films with a thickness of up to 5 layers. Even though those films show liquid-like mobility of the molecules, the structures turn out to remain stable on the time scales of days. Additionally, the properties of the films are studied when heated into the nematic and isotropic temperature range of the bulk material. For films with a thickness of only one smectic layer, a suppression of the nematic phase is observed, whereas the other films exhibit a shift of the phase transition temperature.

CPP 19.9 Tue 18:00 P2

Single Molecule Studies in Liquid Crystals — •Martin Pumpa and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig

Liquid crystals show strong orientational order along a certain director, while lacking spatial order of their centers of mass. For uniaxial liquid crystals the orientational properties lead to anisotropy in the mobility and the optical properties of the material. Recent optical studies focus on their bulk behavior or the diffusion of microscopic particles, gaining only limited information on the microscopic dynamics in the liquid crystal. Single molecule fluorescence detection is in principle able to take a deeper look inside these systems, however, only few single molecule experiments have been published so far.

Here, we compare fluorescence depolarization experiments and single molecule tracking to get the anisotropic mobility of a fluorescent tracer molecule in LC samples. With polarization contrast images we are able to correlate findings from these experiments with the director orientation in the observed areas. Our results deviate strongly from recently published NMR results on the self-diffusion in liquid crystals. Thus we suggest based on additional FRAP measurements a strong influence of the fluorophore on the director structure in its immediate surrounding. This results in a smaller diffusion coefficient due to higher effective viscosities along and perpendicular to the macroscopic director orientation.

CPP 19.10 Tue 18:00 P2

A new method to characterize surface texture via observation of single molecules in video microscopy — •Mario Heidernätsch and Günter Radons — Chemnitz University of Technology, D-09126 Chemnitz, Germany

Single molecule video microscopy is a widely used tool to investigate the dynamic properties of thin liquid films. By analyzing the distribution of diffusivities [1], i.e. the local displacements obtained from the trajectories of the observed dyes, the influence of local inhomogeneities on the diffusion can be revealed. Especially in ultra-thin liquid films the local surface texture strongly influences the diffusivities, thus the resulting diffusion coefficient becomes spatial dependent. We present a new method, the so called diffusion map, which can be easily obtained either from the observed trajectories or, without the necessity of tracking, directly form the recorded videos. We can show that this diffusion map is an indirect representation of the surface texture.

[1] M. Bauer, M. Heidernätsch, D. Täuber, C. von Borczyskowski, G. Radons, Diffusion Fundamentals III **11** (2009), pp. 70.1-70.2

CPP 19.11 Tue 18:00 P2

Bio-chemical functionalization of silicon surfaces — •Lotta Römhildt[1], Claudia Kühn[1], Jörg Opitz[1,2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]Fraunhofer Institute IZFP Dresden, 01109 Dresden

Functionalization of the inorganic interface in nano-bio hybrid materials is a key step for a successful combination of silicon technology at the nanoscale with the specificity of biomolecular recognition in biological systems. The aims are to provide the desired functional groups for the covalent attachment of biomolecules, to guarantee the functionality of the bound biomolecules and to prevent unspecific attachment to the surface. Monolayers on silicon wafers were prepared by covalently binding organic molecules to the surface, such as organosilanes or alkenes, respectively. Biomolecules such as single-stranded DNA are acting as receptors for target molecules. They were further linked to this functionalized surface by using wet bio-chemistry. Static contact angle measurements for the quantification of the wetting behavior indicate that different molecular layers were successfully attached to silicon surfaces. The layer thickness and quality of the film formation were studied with ellipsometry and AFM. Functional end groups like the amino group and potential biomolecules such as DNA strands were labelled with fluorescent dyes to detect the binding with fluorescence microscopy.

CPP 19.12 Tue 18:00 P2

Atomistic Study of Substrate Effect on Polyelectrolyte Adsorption: Poly(Styrene Sulfonate) Monolayer — •Baofu Qiao, Juan Cerda, and Christian Holm — Institute for Computational Physics, University Stuttgart

All-atom level simulations are preformed to investigate the adsorption of polyelectrolytes, for the first time, onto different (hydrophobic vs. hydrophilic) adsorbing substrate, accompanied by a varied surface charge density. In the present work, poly(styrene sulfonate) (PSS) is employed. It shows that the exclusive presence of the short-range wall potential of van der Waals origin is strong enough to form a PSS adsorption layer. Two kinds of conformations of adsorbed PSS chains are observed. The "laying" PSS chains (flat adsorption layer) dominate, with some PSS chains "dangling" into the above solution, which is consistent with a previous experimental work (S. Block and C. A. Helm, J. Phys. Chem. B 2008, 112, 9318.).

CPP 19.13 Tue 18:00 P2

Impedance Spectroscopy Simulation of Solid Electrolytes — •Manuel Landstorfer[1,2], Stefan Funken[1], and Timo Jacob[2] — [1]Institut für Numerische Mathematik, Universität Ulm, Helmholtzstr. 18 — [2]Institut für Elektrochemie, Universität Ulm, Albert-Einstein-Allee 47

Solid electrolytes are promising functional materials for a wide range of applications, *e.g.* lithium ion batteries, solid oxide fuel cells, sensors or electrochromic devices. One of the main characterization methods of electrolytes is the impedance spectroscopy, in which the cell response to AC conditions is monitored. Besides the classical simulations of impedance spectroscopy, in which the electrolyte is modeled as a RC network, more fundamental studies in terms of transport equations can be performed.

We describe ion transport in a solid electrolyte via an extended Poisson–Nernst–Planck system, which takes into account the finite amount of ion sites. Boundary conditions for the impedance spectroscopy simulations are derived, which incorporate the capacitance of the electrode/electrolyte intermediate layer. It resolves space- and time-dependent the charge region within the solid electrolyte. Using a finite element method (FEM) and Newton's methods to solve the nonlinear partial differential equation system, we present numerical results for various frequencies allowing us to evaluate the system's response in impedance spectroscopy measurements. The AC frequency of purely capacitative behaviour, *i.e.* no double layer formation, is determined by our numerical studies.

CPP 19.14 Tue 18:00 P2

Biomineralisation of iron oxides under lipid monolayers studied by x-ray scattering experiments — •Steffen Bieder[1], Florian Wieland[1], Patrick Degen[2], Michael Paulus[1], Martin Schroer[1], Christoph Sahle[1], Johannes Möller[1], Ralph Wagner[3], Heinz Rehage[2], and Metin Tolan[1] — [1]Fakultät Physik/DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [2]Physikalische Chemie II, TU Dortmund, Otto-Hahn-Str. 6, D-44227 Dortmund — [3]Fakultät Physik, Bergische Universität Wuppertal, Gaußstr. 20, D-42097 Wuppertal

Biomineralisation processes provide composite materials which show hierarchical organization as well as complex and controlled shapes.

The biomineralisation processes in living organisms are controlled by proteins and the environment where the process takes place, e.g., the inner cell or the surface of membranes. We studied the biomineralisation of iron oxide in-situ at the aqueous solution/air interface. As a model system for membranes in living cells we used Langmuir layers consisting of lipids with differently charged headgroups in order to investigate the influence of electrostatic interactions on the mineralisation process. The adsorption of iron oxide at the monolayers was observed by grazing incidence diffraction (GID) and extended x-ray absorption spectroscopy (EXAFS). The GID and EXAFS data show an agglomeration of iron oxides at the monolayers. The coordination of the forming iron oxides were similar to the coordination of lepidocrocite and goethite.

CPP 19.15 Tue 18:00 P2

Solvent mapping in conducting polymer blend films using Scanning Transmission X-ray Microscopy — •Markus Schindler[1], Robert Meier[1], Benjamin Watts[2], Jörg Raabe[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany — [2]Paul Scherrer Institute, 5232 Villigen, Switzerland

Since conducting polymers show widespread application possibilities, such as organic field effect transistors and solar cells, their long-time stability is moreover still a serious concern. Aging can be enhanced due to embedded solvent molecules retained in the polymer matrix of the thin films. The remaining solvent affects the mobility of the polymers leading to an ongoing change of the nanoscopic heterostructure, accompanied by changes in the electrical performance.

For thin conducting homopolymer films our results based on X-ray Spectroscopy show a strong dependence of the remaining solvent amount on the particular polymer-solvent-system. By using spatially resolving Scanning Transmission X-ray Microscopy not only compositional maps of polymer-blend films based on P3HT and PVK were obtained, but also solvent distribution maps revealing preferential domains depending on the majority component. This study is complemented with topology sensitive atomic force microscopy measurements.

CPP 19.16 Tue 18:00 P2

Low temperature sintering of thin film polymer/TiO2 solar cells — •Christoph Fahrenson[1], Sylvia Paul[1], Michael Schröder[3], Silvia Janietz[2], and Dieter Neher[1] — [1]Universität Potsdam — [2]Fraunhofer-Institut für Angewandte Polymerforschung, Golm — [3]Justus-Liebig-Universität Gießen

Hybrid solar cells combine an organic semiconductor with a suitable inorganic semiconductor (ref 1). In addition to studies on the well-known Grätzel cell, combinations of a dense or nanostructured TMO layer with soluble conjugated polymers have been subject to recent investigations. One of the problems in the development of efficient polymer/TiO2 cell is the sintering of TiO2-layer. In most cases, the TiO2 layer is prepared via the sol-gel technique and annealing at high temperatures is needed to transform the amorphous layer morphology into a crystalline nanoporous structure. We present a new method to prepare thin layers from crystalline titania nanoparticles while keeping the processing temperature below 100°C. Interlinkage between the individual TiO2 particle is enforced by illumination with UVC-light. Scanning electron microscope (SEM) is used to image the morphology of the thin nanoporous layers. Solar cells were built with the Titanium dioxide layers sintered at moderate temperatures or after UVC sintering, using different donor polymers. Initial experiments show that cells with UVC-sintered layers show comparable solar cell performances than devices using conventional titania layers.

1.*A. C. Arango, L. R. Johnson, et al., Advanced Materials, 12, (2000).

CPP 19.17 Tue 18:00 P2

Fabrication of metallic nanostructures for surface plasmon induced topography changes in azobenzene polymer films — •Arulmozhi Geetha Loganathan[1], Tobias König[1,2], Jürgen Rühe[1], and Svetlana Santer[2] — [1]Department of Microsystems Engineering (IMTEK), University of Freiburg — [2]Institute for Experimental Physics, University of Potsdam

We report on the construction of photosensitive polymer films with integrated metallic gratings in the form of nano-stripes. The metallic stripes were fabricated by two photon lithography. The procedure consist of two steps: First a polymer nano-structure is generated, followed by evaporation of a metallic layer on top of the nano-pattern. Subsequently, thin photosensitive azopolymer films are deposited on top of the active metallic elements. The metallic structures act as nano-scale antennas, in which surface plasmons are excited during homogeneous irradiation with light of an appropriate wavelength. During irradiation of the surface with homogeneous UV light complex intensity patterns can be excited at the metallic interface. The size of generated intensity pattern is below the diffraction limit and can be adjusted under the influence of external stimuli such as variations of the polarization and/or wavelength of the incoming light. The distribution of surface plasmons can be predicted by using FDTD simulations and compared with experimental results. The evanescent field of the surface plasmons is used to induce topography changes in the azobenzene polymer films.

CPP 19.18 Tue 18:00 P2

Novel structuring routine of PEDOT:PSS applied to organic photovoltaics — •Christopher Birkenstock, Robert Meier, and Peter Müller-Buschbaum — TU München, Physik Department, LS Funkt. Mat., James-Franck-Str. 1, 85748 Garching, Germany

In order to improve device characteristics in organic photovoltaic, nano- and micro-structured substrates and polymer layers show a promising way to increase efficiency by optimization of light harvesting and charge carrier separation in solar cells. In this work we present a novel micro-structuring method based on wet-imprinting principles, which can be applied on an electron blocking PEDOT:PSS layer as they are used in electronic applications. It is based on different micro-channel polycarbonate molds and it allows a high ratio of reproducibility and an accurate control of the total film-thickness. The influence of the structuring of PEDOT:PSS on the optical absorption and the overall device efficiency for polymeric solar cells based on P3HT:F8BT blends is investigated. The inner film morphology and the surface topography of the blend films are probed. A light trapping effect is obtained, which allows thinner design conceptions and is interesting for better electrical conductivity trough the photoactive film.

CPP 19.19 Tue 18:00 P2

Surface shear viscosity measurements in quasi 2-d systems — •Uli Langer and Thomas M. Fischer — EP V, Uni Bayreuth, Germany

Measuring the surface shear viscosity of monolayers is a very sensitive way of observing changes in the ordering of the particles the monolayers consits of. Due to the high sensitivity of this method one even gets reliable values for the surface shear viscosity of monolayers in the liquid expanded phase. In contrary to passive microrheology where sensitivity is proportional to the time used for measuring, the measurements with active microrheology take less than a minute.

CPP 19.20 Tue 18:00 P2

Sub-microscopic changes in COP surface properties due to different surface activation processes — •Martin Laher and Sabine Hild — Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstrasse 69, 4040 Linz

Even though the ongoing demand to substitute different materials for polymers due to low cost and mass producibility encouraged lots of studies in polymer science, several questions are still unsolved. A major concern of research is to understand, improve and adjust material properties for specific applications. The substitution of glass or mica with polymers for biological application involves the disadvantage of low surface energy of polymers. The motivation for surface treatments is to adjust surface properties required to improve bonding processes with other polymers. Changes caused by different types of surface modification can increase the surface energy of nonpolar polymers or decrease the glass transition. Due to plasma activation or solvent treatment processes, modifications of mechanical properties like adhesion, stiffness or Young*s modulus of cyclo-olefin-polymer (COP) are expected as well as changes in the microstructure and the hydrophobicity. Surface characterization by means of SFM techniques such as force-distance measurements and SFM-Nanoindentation testing are to be sensitive tools to investigate changes in mechanical properties of polymeric materials. The main challenge is to approve the applicability of provided sensitivity ranges of these methods to detect surface treatment induced changes in the nanometer surface range. Therefore, surface properties of COP samples have been investigated.

CPP 19.21 Tue 18:00 P2

The structure of the interface between a solid substrate and a supercritical gas — •Sebastian Holz, Julia Nase, Michael

Paulus, and Metin Tolan — Fakultät Physik/DELTA, TU Dortmund, 44221 Dortmund

Adsorption at interfaces is critical for many processes in nature, e. g. formation of gas hydrates, catalysis, or industrial applications like water purification. The formation of an adsorption layer enhances the gas offer significantly and is thus of importance for transport and exchange processes at membranes and interfaces in nature. More than 100 models have been established to describe the various types of adsorption isotherms. Supercritical adsorption, however, is far less understood, though this phenomenon has been known for some time now. It has tremendous importance in industrial applications like high pressure gas storage systems, Supercritical Fluid Chromatography (SFC), and polymer processing. However, the interface with a possible restructuration of the supercritical molecules has never been directly measured. In particular, the exact density profile along the surface normal can be determined by x-ray reflectometry, a reliable and well adapted technique to determine the thickness and roughness of interfaces.

We report on preliminary results concerning the adsorption of supercritical carbon dioxide and methane on a silicium wafer. The critical point of carbon dioxide is at T = 304,1 K and p = 73,8 bar and of methane at T = 190,6 K and p = 46,1 bar. We present a new measurement environment meeting the demands of this experimentally difficult study.

CPP 19.22 Tue 18:00 P2

The mesoscopic structure of liquid–vapour interfaces — •Felix Höfling and Siegfried Dietrich — Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, 70569 Stuttgart, and Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

The interfacial region between coexisting phases, e.g., between liquid and vapour, is broadened and roughened by thermal fluctuations. The spectrum of these fluctuations diverges for large wavelengths according to the phenomenological capillary wave theory (CWT). Deviations from CWT have been predicted by density functional theory for inhomogeneous fluids [1]. In particular, an enhancement of fluctuations at mesoscopic wavenumbers is expected due to the long-ranged nature of the intermolecular dispersion forces.

We have performed extensive molecular dynamics simulations for a simple liquid of up to one million particles interacting via a truncated Lennard–Jones potential. Macroscopic properties such as the interface width and the surface tension have been determined and their dependence on system size and cutoff radius of the potential is discussed. Further, the interface structure as encoded in the position-dependent density-density correlation function $H(z_1, z_2, k)$ is analysed. A factorisation property is tested on the obtained data and the wavenumber-dependent surface tension is extracted. Finally, we will address consequences of an external gravitational field on the interface structure.

[1] K. Mecke and S. Dietrich, Phys. Rev. E **59**, 6766 (1999).

CPP 19.23 Tue 18:00 P2

Mesoscopic simulation of multiphase fluid dynamics: interfacial phenomena at pore scale — •Marta S. de La Lama, Stephan Herminghaus, and Martin Brinkmann — Max-Planck-Institute for Dynamics and Self-Organization, Göttingen, Germany

The wide range of length scales involved in multiphase flow points to mesoscale algorithms that capture the relevant physics and coarse-grain the irrelevant atomistic details. The term Multiparticle Collision Dynamics (MPC) comprises a variety of particle-based algorithms which employ successive free-streaming and local multi-particle collision steps [1]. Such collisions are carried out by performing rotations of particle velocities in predetermined cells in a manner that conserves mass, momentum and energy.

The algorithm can be adapted for modeling of multicomponent mixtures [2], and we employ it to analyze interfacial phenomena at pore scale. For instance, we can vary the wetting conditions in slit-pores or observe the effect of heterogeneous wettability on capillary imbibition. Furthermore, MPC is well-suited for complex geometries and, on the other hand, it accounts for thermal fluctuations. This gives us the chance of dealing with more realistic systems. For instance, we analyze how capillary bridges may affect the flow in poly-disperse mesoscopic porous media, what could help to elucidate and optimize the underlying mechanisms that take place in oil-reservoirs and filter materials.

References: [1] G. Gompper et al. ,Adv. Polym. Sci. 221 ,1 (2009) [2] Y. Inoue et al. ,J. Comp. Phys. 201 ,191 (2004)

CPP 19.24 Tue 18:00 P2

The determination of intrinsic interfacial molecules — •Sofia Kantorovich[1,2], Marcello Sega[1], and Pal Jedlovszky[3] — [1]ICP, Universität Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart Germany — [2]USU, Lenin av. 51, Ekaterinburg, 620000 Russia — [3]EKF Department of Chemistry, H-3300 Eger, Leanyka u. 6, Hungary

The identification of molecules or atoms belonging to an interface has been a task of primary importance in many fields, from the case of single molecules to that of liquid-vapor and liquid-liquid interfaces. In the work of Jorge et al. [M. Jorge et al., J. Phys. Chem. C 2010] a comparative analysis showed that the ITIM algorithm [L.B. Partay et al., J. Comput. Chem. 2008], based on a ray-tracing approach, is nowadays the best compromise between speed and accuracy. All the method investigated share the drawback of being primarily developed for the analysis of planar-like liquid-liquid or liquid-vapor interfaces. Here we adopt the concept of weighted alpha-shapes as a tool for identifying interfacial molecules between different phases, independently on the geometry of the interface. We investigate the applicability and computational performances of this approach, and the possibility of its implementation in periodic boundary conditions. Examples of molecular systems with different geometry (planar, spherical and cylindrical) are shown, and in the case of planar interfaces, we provide comparison to the ITIM method. This findings of the study might be used to analyze the interfaces and interfacial properties of systems of physical, chemical and biological interest at different scales.