CPP 79: Wetting, Microfluidics and Confined Liquids II

Time: Friday 9:30–11:30   Location: PC 203

CPP 79.1   Fri 9:30   PC 203

Water Mobility in the Interfacial Quasi-Liquid Layer of Ice/Clay Nanocomposites — •Markus Mezger[1,2], Hailong Li[2], Julian Mars[1,2], Henning Weiss[2], and Wiebke Lohstroh[3] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz — [3]Heinz Maier-Leibnitz Zentrum, Garching

At solid/ice interfaces, a quasi-liquid premelting layer is formed at temperatures below the melting point of bulk water. The water mobility within this premelting layer in ice/clay nanocomposites was determined by quasi elastic neutron scattering. Connections between the translational diffusion coefficient D_t and the surface properties were studied for three clays, serving as model systems for permafrost. Below the bulk melting point, a rapid decrease of D_t is found for all systems, reaching plateau values below $-4\,°C$. At this temperature, D_t in the premelting layer is reduced up to a factor of two compared to super cooled bulk water. Adjacent to charged vermiculite the lowest water mobility was observed, followed by kaolin and the more hydrophobic talc.

CPP 79.2   Fri 9:45   PC 203

Dynamic activity of water confined in hydrophobic and hydrophilic pores probed by neutron spectroscopy — •Margarita Russina[1], Veronika Grzimek[1], Moritz-Casper Schlegel[1,2], and Anita Petrova[1,3] — [1]Helmholtz Zentrum Berlin für Materialied und Energie, Hahn-Meitner Platz 1, 14109 Berlin — [2]BAM Federal Institute for Materials Research and Testing, Unter den Eichen 87, 12205 Berlin , Germany — [3]Saint-Petersburg State University , Faculty of Physics, Petrodvorets, Ulyanovskaya str., 1, Saint-Petersburg, Russia, 198504

The understanding of hydrogen bonds formation in various environment and criteria governing the molecular mobility at nanoscale is of high importance to various fields of applications. Using neutron spectroscopy as a powerful nanoscope we have investigated molecular dynamics of water in hydrophobic and hydrophilic nanoconfinement in a very broad temperature range of 20-300 K. By an aimed selection of the confining systems we were able to follow the molecular behavior in pores of various sizes and in environments with variable degrees of water - host interactions. Changing the amount of confined water allowed us an additional systematic insight. Thus, in hydrophobic zeolite AlPO4-5 we have found pronounced adsorption induced structural contraction as a result of guest-host interactions. Furthermore, with the evolution of the growing water network and increasing guest-guest interactions we observe non-linear changes of the mean square displacement, experimentally determined on the picosecond time scale.

CPP 79.3   Fri 10:00   PC 203

Structure and Dynamics of Confined Liquids Studied by an X-ray Surface Force Apparatus — •Henning Weiss[1], Hsiu-Wei Cheng[2], Julian Mars[1,3], Claudia Merola[2], Veijo Honkimäki[4], Markus Valtiner[2], and Markus Mezger[1,3] — [1]Max Planck Institut for Polymer Research, Mainz, Germany — [2]TU Wien, Institute for Applied Physics, Wien, Austria — [3]Johannes Gutenberg University Mainz, Institute of Physics, Mainz, Germany — [4]ESRF-The European Synchrotron, Grenoble, France

Structure and dynamics of confined liquids were probed by an in-situ X-ray surface force apparatus in plane-cylinder geometry. Our novel device can shear and compress/decompress soft matter within a precisely controlled slit pore confinement. Complementary structural information is obtained by X-ray scattering and simultaneous force measurements. Here, we present results on the structural relaxation of confined liquid crystals (LCs) as reaction to external stimuli. For the smectic LC 8CB we investigated defect-formation and relaxation processes during subsequent compression and decompression cycles. In the second example, an 80 nm thin film of the wet ionic liquid $[C_{10}mim]^+$ $[Cl]^-$ in the columnar LC phase was sheared. The observed mesoscopic orientation induced by oscillatory shear is explained by the anisotropic mobility of the mesogens.

CPP 79.4   Fri 10:15   PC 203

Influence of the ordering of depletants on structural forces in thin liquid films — •Michael Ludwig[1], Sebastian Schön[2], and Regine von Klitzing[1] — [1]Technische Universität Darmstadt — [2]Technische Universität Berlin

Structural forces are observed when pure solvents and ionic liquids, as well as dispersions containing nanoparticles, micelles, polymers or polyelectrolytes are confined between two smooth surfaces. Upon surface-approach, liquid matter has to be depleted from the vicinity of the surfaces, altering the interactions between the surfaces.

Recent experimental studies reveal the superposition of structural forces with DLVO-type forces [1,2]. Here, we will focus on nanoparticle dispersions in confinement between two charged silica-surfaces, as probed in our experiments using a colloidal-probe atomic force microscope (CP-AFM). An additional repulsive term has to be introduced to accurately fit experimental data. This additional term will be discussed in terms of the DLVO-framework.

At high concentrations of depletants, structural force profiles appear to show oscillatory behaviour. The corresponding wavelength λ correlates with the mean particle distance of the depleting particles in the bulk liquid [3]. Different dependencies between wavelength λ and particle number density ρ will be presented considering the bulk liquid geometries.

[1] S. Perkin et al., Phys. Rev. Lett. 119, 026002 (2017) [2] G. Trefalt et al., Phys. Rev. Lett. 177, 088001 (2016) [3] R. von Klitzing et al., Soft Matter 7, 10899 (2011)

CPP 79.5   Fri 10:30   PC 203

Non-equilibrium surface critical dynamics in a confined binary liquid mixture — •Sutapa Roy[1], Felix Höfling[2], and Siegfried Dietrich[1] — [1]Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany and Institute for Theoretical Physics IV, University of Stuttgart, Germany — [2]Freie Universität Berlin, Department of Mathematics and Computer Science, Berlin, Germany

Close to a solid surface the static and dynamic properties of a fluid deviate significantly from their bulk behaviour. In this context, by using molecular dynamics simulations, we investigate the rich non-equilibrium relaxation dynamics of a binary liquid mixture [1] confined to a slit pore, fully respecting hydrodynamic conservation laws. A sudden temperature quench of the liquid from the disordered phase to its bulk demixing critical point yields a non-equilibrium response. The corresponding dynamics, characterised by the two-time auto-correlator of the position-dependent order parameter, exhibits aging and scaling [2]. Analysis of the aging behaviour allows us to quantify the crossover from surface- to bulk-like dynamics. Our results for the surface adsorption profiles in equilibrium are compared with recent theoretical predictions for the canonical ensemble [3]. To the best of our knowledge, this study is the first one to explore both surface and bulk *aging* phenomena of a liquid at criticality.

[1] S. Roy, S. Dietrich & F. Höfling, J. Chem. Phys. **145** 134505 (2016). [2] S. Roy, F. Höfling & S. Dietrich, unpublished (2017). [3] M. Gross, O. Vasilyev, A. Gambassi & S. Dietrich, Phys. Rev. E **94** 022103 (2016).

CPP 79.6   Fri 10:45   PC 203

Electrolyte solutions confined by non-uniform walls — •Maximilian Mussotter and Markus Bier — Max-Planck Institut für Intelligente Systeme und Universität Stuttgart, 70569 Stuttgart, Germany

In contrast to fluids comprising electrically neutral constituents and uncharged walls, the widely used assumption of substrates with uniform wall-fluid interactions is questionable beyond molecular length scales in the context of charged substrates and dilute electrolyte solutions, where the influence of non-uniformities can be on the scale of the Debye length. For this reason the goal of this work was to deepen understanding of electrolyte solutions in contact with non-uniformly charged substrates. The system is studied by means of classical density functional theory, within the framework of square-gradient and double-parabola approximation. This work is intended to lay the foundations for future studies of fluids confined by non-uniform boundaries.

CPP 79.7   Fri 11:00   PC 203

Metadynamics calculation of chemical potential in dense and confined fluids — •Claudio Perego[1] and Michele Parrinello[2] — [1]Max Planck Institute for Polymer Research, Mainz (De) — [2]Swiss

Federal Institute of Technology, Zurich (Ch)

Chemical potential is a crucial thermodynamic quantity, regulating phase and chemical equilibria in a wide range of systems. The calculation of chemical potential in dense fluids represents a long-standing challenge in molecular simulations. An established approach builds on Widom's method, in which chemical potential is computed by sampling the insertion energy of a test particle. The resulting value is mostly determined by low energy insertions, in which the test particle is placed in a proper cavity within the system particles. In dense liquids such cavities are rarely available, and the sampling is restricted to large insertion energies, preventing the convergence of the estimate. Here we present a new method for computing the chemical potential in dense liquids. The technique builds on metadynamics to extend the insertion energies to the relevant low energy region, inaccessible in unbiased simulations. We show that the method can be also generalized for the computation of chemical potential in non-homogeneous fluids, which represents a crucial step for the study of nano-fluidics and confined liquids. The technique is then tested with both homogeneous and non-homogeneous Lennard-Jones fluids. As a result accurate chemical potential estimates are obtained even at large densities, where the classical approach fails.

CPP 79.8   Fri 11:15   PC 203

Heisenberg fluids under confinement — •Stefanie Maria Wandrei[1], Roland Roth[2], and Martin Schoen[1] — [1]Technische Universität Berlin — [2]Eberhard Karls Universität Tübingen

In this work we employ classical density functional theory (DFT) to investigate the behavior of a Heisenberg fluid at a single wall or confined to a nanoscopic slit pore of variable width. We consider three different types of confining surfaces: hard walls, simple attractive walls, and attractive walls with an additional field acting on the spins. To account for the locality of the density we use the White Bear version of fundamental measure theory. This allows us to investigate in greater detail than in previous works the effect that competing external fields have on the behavior of the confined fluid.