CPP 43: Wetting, Fluidics and Liquids at Interfaces and Surfaces (joint session CPP/DY)

Time: Thursday 15:00–17:30   Location: H 0107

CPP 43.1   Thu 15:00   H 0107

Dynamic wetting of concentrated granular suspensions — •Reza Azizmalayeri, Peyman Rostami, and Günter K. Auernhammer — Leibniz-Institut für Polymerforschung, Dresden, Germany

Concentrated granular suspensions are employed in a variety of applications in which the contact line dynamics and internal structure of the suspension interact. The process can be characterized using individual particle analysis and average suspension descriptions. There is a markedly high shear rate at the droplet's contact line. This localized shear rate profoundly affects the suspension's non-Newtonian rheological behaviour. Recent researches have affirmed the applicability of hydrodynamic solutions like Cox-Voinov relation to granular suspensions. Despite these efforts, the impact of particles on the overall flow field and microstructure of densely packed granular systems along the contact line remains unexplored. In this study, a configuration consisting of a pinned droplet on a moving substrate is utilized. Using astigmatism particle tracking velocimetry (APTV), we precisely track the 3D motion of tracer particles within the suspension. Near the advancing contact line, we observe distinct behaviours based on the interaction between particles. A concentrated suspension of low interacting particles violates the Cox-Voinov relationship with particle friction becoming a significant factor. Meanwhile, when strong particle interactions are present the suspension exhibits a yield stress behaviour. The receding contact line exhibits a dynamic curvature that undergoes a transient phase before reaching a stationary state. The results of this study are supported by rheology measurements.

CPP 43.2   Thu 15:15   H 0107

How rheology influences the wetting behavior of droplets — •Günter K. Auernhammer[1], Peyman Rostami[1], Reza Azizmalayeri[1], Valentine Comoy[1], and Mathis Fricke[2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Department of Mathematics, TU Darmstadt, Germany

We study the spreading of viscous and viscoelastic drops on solid substrates with different wettability. In the early stages of spreading, we find that the viscoelastic drop spreads with faster and a different power law than the Newtonian drop (i.e. aqueous glycerine solution) for the same zero shear rate viscosity. We argue that the effect of viscoelasticity is only observable for experimental time scales in the order of the internal relaxation time of the polymer solution or longer times. Near the contact line, the effective viscosity is lower for the viscoelastic drop than for the Newtonian drop. Together with its shear rate dependency, this difference in effective viscosity can explain the different spreading dynamics. We support our experimental findings with a simple perturbation model that qualitatively agrees with our findings. [https://arxiv.org/abs/2308.14515]

CPP 43.3   Thu 15:30   H 0107

Surface Sensitive Fractioning of Microparticles and Microplastics — •Marek Bekir — Institut für Physik und Astronomie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

Separation of particles of equal size but different surface energies is nowadays a challenging task. With local-light driven diffusioosmosis (local-LDDO) [1] in combination with microfluidic technology [2] we provide a potential tool for separation of such microparticles and microplastics. The local-LDDO is a phenomenon of a photosensitive azobenzene containing surfactant, where under illumination a dynamic exchange of isomers provides a repulsive flow strong enough to elevate particles up to several micrometers from the liquid-glass interface of the microfluidic chamber. In combination of a superimposed lamellar fluid flow the elevation leads to a stronger passive motion along the streamline. We demonstrate that the lift off depends on the size but also on the surface morphology, surface material and surface coating, too, i.e. differently surface modified particles therefore a different motion velocity.[3]

[1] Feldmann, D.; Arya, P.; Molotilin, TY.; Lomadze, N.; Kopyshev, A.; Vinogradova, OI.; Santer, S. Langmuir 2020, 36, 6994-7004.

[2] Sajeesh, P.; Kumar Sen, A. Microfluid Nanofluid 2014, 17, 1-52.

[3] Bekir, M.; Sperling, M.; Vasquez Muñoz, D., Braksch, C.; Böker, A.; Lomadze, N.; Popescu, M. N., Santer, S. Advanced Materials 2023, 35, 2300358.

CPP 43.4   Thu 15:45   H 0107

Curvature-dependent adsorption of surfactants in water nanodroplets: Insights from molecular dynamics — •Fabio Staniscia and Matej Kanduč — Department of Theoretical Physics, Jožef Stefan Institute, Ljubljana SI-1000, Slovenia

Adsorption of surfactants at curved air-water interfaces plays a major role in phenomena involving nanodroplets, such as emulsification, wetting, heterogeneous catalysis, and aerosol chemistry. Once the nanodroplet becomes small enough, its large curvature can influence the adsorption of surfactants, which has not been thoroughly investigated. At this scope we investigate the adsorption of short-chain surfactants inside water nanodroplets using molecular dynamics simulations. We show that the curvature of the droplet interface enhances adsorption and affects other interfacial properties, such as the preferred surfactant orientation. We relate this behavior to curvature-dependent surface tension of water, described by the Tolman length correction. We show that the influence of curvature on adsorption grows exponentially with the size of the hydrophobic tail of the surfactant. Finally, we use our theoretical model to predict the behavior of larger surfactants and of larger droplets.

CPP 43.5   Thu 16:00   H 0107

Interfacial versus confinement effects in the frequency dependent dielectric response of nanoconfined water — •Maximilian Becker and Roland R. Netz — Freie Universität Berlin, Berlin, Germany

We investigate the frequency-dependent dielectric response of water confined between two graphene sheets with force-field and density-functional-theory based molecular dynamics simulations. We highlight the critical role of the volume over which the dielectric response is averaged when measuring the dielectric susceptibility and introduce a system-size-independent decomposition, allowing us to discern interfacial and confinement contributions to the overall dielectric spectrum. Using this, we discuss the molecular origin of the main absorption features of nanoconfined water from the GHz to the THz regime: While intermolecular orientational correlations govern the interfacial and confinement effects on the 30 GHz Debye peak and the static dielectric constant, the 20 THz librational peak undergoes intensity changes which can be attributed to a change in single-molecule motion. When going from bulk to confinement, DFT-MD simulations reveal the emergence of a broad spectroscopic band arising between 1 and 30 THz, a region which is known to probe the dynamics of hydrogen bonds in water. These results are interpreted in the context of the hydrogen bond network at the water-graphene interface and in two-dimensional water layers which sheds light on the intricate behavior of water molecules within confined environments and contributes to a deeper understanding of their dielectric properties.

30 min. break

CPP 43.6   Thu 16:45   H 0107

Improved displacement efficiency in Ganglia size distribution by invasion of complex fluids — Karthik Nuthalapati[1] and •Ralf Seemann[2] — [1]Universität des Saarlandes, Saarbrücken, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

It is well-known that the viscoelastic nature of polymer solutions affects the displacement process when used as displacing fluids, for example, in enhanced oil recovery. Nevertheless, the microscopic displacement efficiency within porous media remains elusive. In this study, we experimentally investigated the impact of polymer viscosity and elasticity on the displacement efficiency of silicone oils with different viscosities. As displacing fluids, we explored four types of complex fluids, including a highly viscous Newtonian fluid, a shear-thinning solution with negligible elasticity, an elastic polymer with constant viscosity, and a viscoelastic polymer solution made from a polyelectrolyte within the Ganglia size distribution. As a result, viscoelastic polymers demonstrated improved displacement efficiency in Ganglia size distribution through the invasion of complex fluids.

CPP 43.7   Thu 17:00   H 0107

The Structure of Water Under Confinement in Periodic Mesoporous Organosilicas Investigated by X-Ray Scatter-

ing — •Niels Christian Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Tamás Simon[2], Wonhyuk Jo[1,4], Nele Naomi Striker[1], Michael Fröba[2,3], and Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Institute of Inorganic and Applied Chemistry, Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [4]European XFEL, Schenefeld, Germany

The effect of pore wall chemistry and pore diameter on the structure of confined water was studied by X-ray scattering on water confined in periodic mesoporous organosilicas (PMOs). A shift in the first structure factor peak at $q \approx 1.8$ Å^{-1} reveals a variation in the density of the confined water in dependence of hydrophilicity and pore size. Smaller and more hydrophilic pores induce a lower density in the water. In contrast to bulk water, the pair distribution functions (PDFs) of confined water show a splitting of the second-neighbour peak into either two, in the case of smaller and more hydrophilic pores, or three separate peaks, in larger and more hydrophobic pores. From the running coordination number we conclude that smaller and more hydrophilic confinement leads to a stronger developed tetrahedral network in confined water, while confinement in larger and hydrophobic pores give tetrahedral arrangements that are bulk-like or even less pronounced than in bulk water.

CPP 43.8   Thu 17:15   H 0107
Unveiling the Role of Surface Hydrophobicity and Defects in Heterogeneous Cavitation by Atomistic Simulations —
•Philip Loche[1,2], Matej Kanduč[3], Emanuel Schneck[4], and Roland R. Netz[2] — [1]EPFL, Lausanne, Switzerland — [2]FU Berlin — [3]Jožef Stefan Institute, Ljubljana, Slovenia — [4]TU Darmstadt, Darmstadt, Germany

The reduction of pressure in liquids can lead to vaporization and the formation of bubbles, a phenomenon known as cavitation. Cavitation is commonly observed in hydraulic machinery, ship propellers, and even within biological systems. Liquids can sustain enormous negative pressures until reaching their stability limits, at which point cavitation occurs. While classical nucleation theory well explains the energetics of these events, little is known about the dynamics of interfacial bubble formation.

We quantify the kinetics of heterogeneous cavitation using classical nucleation theory and atomistic simulations of self-assembled monolayers at various contact angles under a constant rate protocol. Our focus is on the impact of surface hydrophobicity and defects. We find that increased hydrophobicity leads to a predominance of heterogeneous cavitation at surfaces. Simulations reveal an exponential relationship between the contact angle and the kinetic prefactor, with heightened hydrophobicity significantly reducing this parameter. The balance pressure, where homogeneous and heterogeneous cavitation rates converge, indicates a critical contact angle for switching between these two effects under realistic pressures and volumes.