

CPP 47: Wetting, Droplets, and Microfluidics (joint session DY/CPP)

Time: Thursday 15:00–17:45

Location: BH-N 334

CPP 47.1 Thu 15:00 BH-N 334

Structure Formation in Supraparticles Composed of Spherical and Elongated Colloidal Particles — YASHRAJ M. WANI¹, MELIS YETKIN², ●KRITIKA KRITIKA^{1,3,4}, MICHAEL HOWARD⁵, HANS-JÜRGEN BUTT², MICHAEL KAPPL², and ARASH NIKOUBASHMAN^{1,3,4} — ¹Johannes Gutenberg Universität Mainz — ²Max-Planck-Institut für Polymerforschung — ³Leibniz-Institut für Polymerforschung — ⁴Technische Universität Dresden — ⁵Department of Chemical Engineering Auburn University

In the present work, we use experiments and computer simulations to investigate the formation of supraparticles (SPs) through the evaporation-driven assembly of spherical and elongated colloidal particles (CPs). We systematically explore how different aspect ratios ($\lambda=4,6,11$) of the CPs and the drying conditions influence the final morphologies of SPs. In the evaporation-limited regime, where the rate of CP advection is much larger than the rate of CP diffusion, we find a short-ranged orientational ordering of the CPs on the SP surface and isotropic packing in the core. In contrast, simulations in the diffusion-limited regime show a long-ranged orientational ordering of the rods on the SP surface and local nematic ordering in the core. Additionally, we explore SPs fabricated from rod-sphere mixtures, where a thin shell of rods was observed for the slowly dried SPs. In all cases, we also observe that the porosity of the SPs increases with increasing aspect ratio of the elongated CPs.

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Investigation of nonlinear electrophoresis in microfluidics with alternating voltages — ●ROBERT EPKENHANS¹, RALF EICHORN², DARIO ANSELMETTI¹, and MARTINA VIEFHUES¹ — ¹Bielefeld University — ²Nordita Stockholm

Electrophoresis (EP) is a common phenomenon in microfluidics used for controlled migration of biomolecules like DNA or for size selective migration in gels. In the linear, low-field regime the EP-mobility is dependent only on the particle-zeta and the ambient electrolyte. Yet, recent studies revealed a polynomial velocity increment for colloid particles exposed to high electric fields above roughly 100 kV/m with the underlying physical mechanisms still under debate.

In our studies, we quantified the nonlinear response in the mobility of charged particles in a microfluidic PDMS-chip as a function of the applied electric field strength. Therefore, we used 1) a superimposition of low DC-fields (0-13 kV/m) and high sinusoidal alternating fields up to 260 kV/m, 2) asymmetric potentials yielding a vanishing time-averaged mean, but non-vanishing higher-order mean value. We present several data sets for the particle velocities with a variation of ionic concentration and types and the respective higher-order electrophoretic mobilities. Our results suggest that nonlinear-EP forces are rather relevant in insulator-based microfluidics instead of dielectrophoresis. This opens new possibilities for particle separation devices, e.g. DNA-molecules, since the up to date data indicates size- and shape-dependent electrophoresis in the nonlinear regime. Concerning these matters, we provide suggestions for future studies on nonlinear electrophoresis.

CPP 47.3 Thu 15:30 BH-N 334

Dynamic density functional theory for drying colloidal suspensions: Hydrodynamic interactions in spherical confinement — ●MAYUKH KUNDU¹, YASHRAJ M. WANI², KRITIKA KRITIKA^{2,3,4}, ARASH NIKOUBASHMAN^{2,3,4}, and MICHAEL P. HOWARD¹ — ¹Department of Chemical Engineering, Auburn University, Auburn, USA — ²Institute of Physics, Johannes Gutenberg University, Mainz, Germany — ³Leibniz-Institut für Polymerforschung Dresden, Germany — ⁴Institut für Theoretische Physik, TU Dresden, Germany

We investigate the role hydrodynamic interactions (HI) play in the evolution of structures in one-component drying colloidal suspensions confined within spherical droplets. We develop a continuum model for the distribution of hard-sphere particles in the droplet based on dynamic density functional theory (DDFT). To compute the particle flux during drying, we employ an accurate free-energy functional based on fundamental measure theory (FMT) in conjunction with pairwise far-field HI described by the Rotne-Prager-Yamakawa (RPY) mobility tensor. To validate the DDFT model, we compare the DDFT predictions with particle-based Brownian dynamics (BD) and multiparticle

collision dynamics (MPCD) simulations in selected cases. We also compare our model to DDFT and particle-based models, including only free-draining HI, in order to systematically characterize the effects of HI between particles. Our work illustrates the importance of including HI in models of nonequilibrium self-assembly processes such as drying and demonstrates a systematic way of constructing such models.

CPP 47.4 Thu 15:45 BH-N 334

Numerical study of evaporation-driven particle deposition on a substrate — ●QINGGUANG XIE¹ and JENS HARTING^{1,2} — ¹Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IEK-11), Forschungszentrum Jülich GmbH, Erlangen, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Deposition of functional materials on a substrate is a vital process in printing and coating technologies, playing important roles in numerous applications such as photovoltaics, lithium batteries, and electrolyzers. The structure of the deposition is crucial for device performance; however, our understanding of the deposition process is still lacking. We conducted numerical studies on the particle deposition process. Initially, we developed a diffusion-dominated evaporation model using a multicomponent lattice Boltzmann method. We validated the applicability of our model by demonstrating agreement in the time evolution of the interface position of an evaporating planar film and a freely floating droplet with analytical predictions. Subsequently, we investigated the deposition of particles on a substrate by drying a colloidal suspension droplet. We explored, both numerically and theoretically, the effect of friction between the particles and the substrate on the deposition pattern. With an increase in friction force, we observed a transition from a dot-like to a ring-like deposit. More recently, we studied the effect of van der Waals force between particles and substrate wettability on the deposition pattern when drying a thin film. We proposed a strategy to achieve highly uniform deposition.

CPP 47.5 Thu 16:00 BH-N 334

Coalescence of biphasic droplets embedded in free-standing smectic A films — ●CHRISTOPH KLOPP¹, TORSTEN TRITTEL², and RALF STANNARIUS¹ — ¹Otto von Guericke Universität Magdeburg, Institut für Physik, ANP — ²TH Brandenburg, Fachbereich Technik

Coalescence of droplets is ubiquitous in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in three dimensions (3D) and on two-dimensional (2D) solid or liquid substrates, e.g. [1-3]. We investigate micrometer-sized flat droplets consisting of an isotropic core surrounded by a nematic rim (biphasic droplets) in freely suspended smectic A liquid-crystal films. In contrast to purely isotropic droplets which are characterized by a sharp edge and no long-range interactions, the nematic rim introduces a continuous film thickness change resulting in long-range mutual attraction of droplets. We show the appearance of a unique structural wall separating the isotropic cores of the droplets during the merging process.

[1] J. D. Paulsen et al., Nat. Commun., 5, 3182 (2014) [2] D. G. A. L. Aarts et al., Phys. Rev. Lett., 95, 164503 (2005) [3] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019)

15 min. break

CPP 47.6 Thu 16:30 BH-N 334

Mutual information as a measure of mixing efficiency in viscous fluids — ●YIHONG SHI — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

Because of the kinematic reversibility of the Stokes equation, fluid mixing at the microscale requires an interplay between advection and diffusion. Here we introduce mutual information between particle positions before and after mixing as a measure of mixing efficiency. We demonstrate its application in a Couette flow in an annulus and show that the mixing efficiency depends in a non-trivial way on the time sequence of rotation. We also determine mutual information from Brownian dynamics simulations using data compression algorithms and demonstrate that advanced neural network based compression algorithms can be applied to estimate mutual information to a high accuracy. Our results show that mutual information provides a uni-

versal and assumption-free measure of mixing efficiency in microscale flows.

CPP 47.7 Thu 16:45 BH-N 334

Leveraging geometry and catalyst distribution to optimize the yield of catalytic microreactors — ●GONCALO ANTUNES¹, PAOLO MALGARETTI¹, and JENS HARTING^{1,2} — ¹Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien, Forschungszentrum Jülich, Erlangen, Germany — ²Department Chemie- und Bioingenieurwesen und Department Physik, Friedrichs-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

We develop a semi-analytical model for transport in heterogeneous catalytic microreactors, where both reactant and product are in the gas phase. Making use of the lubrication and Fick-Jacobs approximations, we reduce the three-dimensional governing equations to an effective one-dimensional set of equations. Our model captures the effect of compressibility, of corrugations in the shape of the reactor, as well as of a non-homogeneous catalytic coating of the reactor walls. We then show how to optimize the output of product by tuning the geometrical and chemical properties of the reactor, such as its length, for which we find an optimum value. We further explore the compressible regime, in which an optimum corrugation height emerges. This height depends on the distribution of catalytic material. Finally, we apply our theory to a model porous material, and find an optimum pore size that maximizes the output of product.

CPP 47.8 Thu 17:00 BH-N 334

Rolle of water accumulation in dynamic friction on hydrophobic surfaces — ●IGOR STANKOVIĆ¹, PIERRE-EMMANUEL MAZERAN², and OLIVIER NOEL³ — ¹Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, 11080 Belgrade, Serbia — ²Sorbonne Universités, Université de Technologie de Compiègne, Laboratoire Roberval, FRE UTC-CNRS 2012, CS 60319, 60203, Compiègne, France — ³IMMM, UMR CNRS 6283, Le Mans Université, Avenue O. Messiaen, 72085 Cedex 09, Le Mans, France

The nature of dynamic friction on water molecule-contaminated surfaces is still poorly understood. The capillary phenomena in tribological contact with graphite, a commonly used material, were investigated using circular mode atomic force microscopy and molecular dynamics simulations. Here, we demonstrate that an intuitive paradigm, which asserts that water molecules are squeezed out of hydrophobic contacts, needs to be refined. Consequently, we introduce a mechanism considering a droplet produced within the sliding nanocontact by the accumulation of water adsorbed on the substrate. Our results show that a full slip regime of the droplet sliding on the hydrophobic substrate explains the experimental tribological behaviour.

References I. O.Noel, P.-E. Mazeran, I.Stanković, ACS Nano 16, 10768-10774 (2022).

CPP 47.9 Thu 17:15 BH-N 334

Active-matter-fueled interfacial microflows — ●KUNTAL

PATEL^{1,2} and HOLGER STARK¹ — ¹Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — ²Max-Planck-Institut für Sonnensystemforschung, Göttingen, Germany

Several chemical and biomedical applications require systematic processing of micron-sized fluid samples. To realize this, so-called microfluidic lab-on-a-chip devices with micron-sized channels are widely used. Often, one needs to manipulate interfaces separating immiscible fluids in such channels. The interface separating the two fluid components costs energy, which is quantified by surface tension. Thus, any deformation of a planar fluid interface increases energy.

In our work, we assign one more property to the interface in the form of dipolar forces acting perpendicular to the interface. We name it the *activity* of the interface, and it is achieved by covering the interface with active particles. The notion of activity is inspired by swimming microorganisms. Using lattice-Boltzmann simulations, we discover that the presence of activity affects the stability of the interface. We notice that dipolar forces pointing towards the interface counter the stabilizing effect of surface tension, so that the interface deforms. In contrast, force components pointing away stabilize the planar interface. We demonstrate that one can leverage such activity-induced instability to generate microfluidic droplets and manipulate liquid sheets. In addition, we can also control droplet formation by varying the magnitude of dipolar forces in real time, which can be accomplished using light-sensitive active particles in practice.

CPP 47.10 Thu 17:30 BH-N 334

Extracting oil from an oil and water mixture by using their different wetting properties via the Acoustowetting phenomenon — ●OFER MANOR — Technion - Israel Institute of Technology, Haifa, Israel

The free surface of an oil in water emulsion usually catalyzes the formation of a thermodynamically favorable oil film far before the emulsion destabilizes in the bulk of the mixture: We stabilize 170 nm nano-emulsions by surfactants—SDS or Tween 20. The emulsions remain stable for 12 months in closed vessels. However, micron thick oil films appear within minutes on 10 micro-liter sessile drops of the emulsions. We extract the micron-thick oil film off the free surface of the emulsion drops using a traveling 20 MHz-frequency surface acoustic wave (SAW) in the solid.

In our experiments, we place drops of emulsion atop a lithium niobate substrate that supports a traveling SAW therein. Oil films leak off the emulsion sessile drops 1-20 minutes from the commencement of the experiment, dynamically wetting the solid under acoustic stress—the Acoustowetting phenomenon. The Acoustowetting phenomenon discriminates between the water and oil phases via their wetting properties: The SAW powers the dynamic wetting of the solid by the oil film, extracting oil mass off the emulsion drops, while keeping the higher surface-energy water phase in place. The thickness of the oil film, leaking off the drops, oscillates between 20 to 1 microns and sustains a crystal-like pattern of lateral micron dimensions and submicron thickness of unknown origin in the presence of the SAW.