CPP 20: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–12:45 Location: ZEU/0160

CPP 20.1 Tue 9:30 ZEU/0160

Process-Directed Self-Assembly of Copolymer Blends: Micro- and Macrophase Separation — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, 37077 Göttingen, Germany

The equilibrium phase behavior of binary diblock copolymer blends involves a complex interplay between microphase and macrophase separation. We investigate blends of linear diblock copolymers, A_1B_1 (cylinder-forming) and A_2B_2 (cylinder- or lamella-forming), using a combination of self-consistent field theory (SCFT) and single-chain-in-mean-field (SCMF) simulations. When the chain-length asymmetry between the A_1B_1 and A_2B_2 copolymers becomes large, the equilibrium phase diagram exhibits a wide macrophase-separation channel. Strikingly, our simulations reveal a strong pathway dependence within this region: rapid quenching yields a spatially homogeneous structure with narrow cylinder-size distributions and strong hexagonal order, whereas gradual annealing promotes local demixing, resulting in bimodal domain sizes and weaker order. We demonstrate that this process-dependent nonequilibrium behavior can be explained by the distinct evolutions of the system state and free-energy landscape of the blends under quenching or annealing. These findings highlight how different processing conditions can direct nanostructure formation in block copolymer blends, and establish a mechanistic link between processing pathway and the final morphology, thus offering insights into rational design of targeted nanostructured materials.

CPP 20.2 Tue 9:45 ZEU/0160

Topological defect engineering enables size and shape control in self- assembly — Lara Koehler[1,3], Markus Eder[2], Vincent Ouzan-Reboul[3], Christoph Karfusehr[2], Andrey Zelenskiy[3], Pierre Ronceray[4], Friedrich Simmel[2], and •Martin Lenz[3] — [1]MIPPKS, Dresden, Germany — [2]TU Munich, Germany — [3]U. Paris-Saclay, Orsay, France — [4]Aix-Marseille-Université, Marseille, France

Equilibrium self-assembly is a powerful way to build nano- and microscale structures out of interacting subunits. The size and shape of such structures must be controlled in many biological and technological functions, posing significant practical challenges as current strategies require multiple subunit types or the precise control of their shape and mechanics. Here we introduce an alternative approach that circumvents these obstacles. Our method uses subunits whose interactions promote crystals, but also favor crystalline defects. We show theoretically that the magnitude of these interactions, which is well controlled in experiments, governs the self-assembly through topological restrictions on the scope of the defects. Using DNA origami, we demonstrate both size and shape control in two-dimensional disk- and fiber-like assemblies. Our basic concept of defect engineering operates well beyond these examples, and provides a broadly applicable framework to control self-assembly.

CPP 20.3 Tue 10:00 ZEU/0160

Soft colloidal monolayers under drying conditions — •Kai Luca Spanheimer[1], Maret Ickler[2], Julian Ringling[3], Nicolas Vogel[2], Matthias Karg[4], and Hartmut Löwen[1] — [1]Insitut für Theoretische Physik II, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Institute of Interfaces and Particle Technology, Friedrich-Alexander University, Erlangen, Germany — [3]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [4]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Langmuir-Blodgett deposition is a well established technique in research and industry. Even though, there still are effects in this process that are not yet explored from a theoretical standpoint. It is usually assumed that the deposited pattern is identical with the one appearing at the water-air interface. In recent experimental studies, strong reorganization during the drying of soft colloidal monolayers has been observed [1]. Capillary forces during drying are known to change nanoscopic structures, sometimes even leading to their destruction. To model these processes we propose a combination of overdamped particle dynamics coupled to dewetting dynamics of an evaporating liquid film. The patterns produced by this model fit those observed in experiment. This theoretical approach allows exploration of the drying dynamics. Thereby we gain new insights into the drying process and makes experimental results produced with Langmuir-Blodgett deposition more reliable.

[1] K. Kuk, et al: Adv. Sci., 11, 2406977 (2024).

CPP 20.4 Tue 10:15 ZEU/0160

Mechanical assessment of microfluidically-generated poroelastic microgel particles — Aude Sagnimorte[1,2], Anke Lindner[2], and •Joshua McGraw[1] — [1]Gulliver-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris — [2]PMMH-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris

Soft microgels have numerous applications in diverse fields,such as tissue engineering, drug delivery systems, soft robotics, or as model systems for suspensions or colloids. Among these, photopolymerized hydrogels such as poly(ethylene glycol) diacrylate (PEGDA) are commonly used due to their highly tunable mechanical properties. However, proper characterisation of these properties is challenging, in part due to their small scale, on the order of tens of microns, and in particular the lack of assessment of their time-dependent properties. Here we provide a comprehensive mechanical characterisation of individual photopolymerised microgels particles using atomic force microscopy (AFM) for precise local measurements. In particular, we performed indentation-relaxation tests on PEGDA microdisks immersed in water. By varying indentation depth and probe diameter, we changed the contact area and observed relaxation responses which are indicative of poroelastic behaviour. In particular, larger contact areas resulted in longer relaxation times. Our results also show that increasing the amount of solvent increased the relaxation time. Our collected results are consistent with a simple, Herzian poroelastic model giving good agreement with both the approach and relaxation phases of the experiments.

CPP 20.5 Tue 10:30 ZEU/0160

Nonlinear Viscoelastic Response and Stress Shielding in Driven Bistable Spring Chains — •Sven Pattloch[1,2] and Joachim Dzubiella[1,2] — [1]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany. — [2]Cluster of Excellence livMatS@FIT-Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-Universität Freiburg, D-79110 Freiburg, Germany

Bistable micromodules are a promising route to design adaptive mechanical metamaterials with tunable viscoelastic response. Here, a driven one-dimensional chain of bistable springs is studied in which both the mechanical deformation and the internal excitation states evolve dynamically under time-dependent forcing. Their coupling produces rich nonlinear viscoelastic behaviour, including frequency-dependent susceptibilities, delayed deformation, and pronounced hysteresis in cyclic loading.

Using analytical linear response theory complemented by numerical simulations, the model quantifies how microscopic parameters and driving protocols control effective stiffness, loss, and phase lags. A key result is a strong attenuation ('shielding') of stress propagation along the chain that is already present for monostable springs but is markedly amplified by excitation switching in bistable modules. These findings provide simple design principles for tailoring nonlinear viscoelasticity, hysteresis, and stress shielding in driven soft matter and mechanical metamaterial systems.

CPP 20.6 Tue 10:45 ZEU/0160

Euler buckling on curved surfaces — •Shiheng Zhao[1,2,3] and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Nearly three hundred years ago, Euler showed that an inextensible straight elastic line in the plane buckles under compression when the compressive force F reaches a critical value $F_* > 0$. But how does such an elastic line buckle within a general curved surface? Here [1], we reveal that the classical instability changes fundamentally: By weakly nonlinear analysis of the buckling of an asymptotically short elastic line, we show that the critical force for the lowest buckling mode is $F_* = 0$ and discover a new bifurcation structure in which the modes of classical Euler buckling split into pairs. For long elastic lines,

we numerically find an additional bifurcation by which the second of these new modes becomes the lowest mode and show that, at sufficiently large F, they undergo discontinuous snap-through to higher end-to-end compression. We explain these bifurcations in terms of the general unfolding of a pitchfork. This constitutes the foundations for a class of mechanical instabilities within curved surfaces from which, for example, biological shape emerges in development.

[1] S. Zhao and P. A. Haas, Phys. Rev. Lett. (in press)

15 min. break

CPP 20.7 Tue 11:15 ZEU/0160

Linking molecular dynamics and experimental FORCs in multicore magnetic nanoparticles — Ekaterina Novak[1], •Malika Khelfallah[2], Andrey Kuznetsov[3], Deniz Mostarac[4], Claire Carvallo[2], Amélie Juhin[2], and Sofia Kantorovich[3] — [1]Ekaterinburg, Russia — [2]Sorbonne Université, Paris, France — [3]University of Vienna, Vienna, Austria — [4]University of Edinburgh, Edinburgh, United Kingdom

Multicore magnetic nanoparticles - clusters of several magnetic grains embedded in a nonmagnetic matrix - exhibit collective behaviour distinct from single-core particles and are promising candidates fro drug targeting and magnetic hyperthermia. Their magnetic cores possess finite anisotropy, and the multicore assemblies range from near-spherical to elongated ellipsoids, features that strongly affect their response to external fields. To study these effects, we use molecular dynamics simulations [1] to model internal structure, anisotropy distribution, and collective switching. As a key diagnostic, we employ First Order Reversal Curves [2], which experimentalists routinely measure for immobilised multicore particles, enabling direct comparison between simulations and experiments. FORC diagrams reveal coercivity distributions and magnetic interactions between grains, offering detailed insight into interaction mechanisms and domain processes.

The work was financially supported by the RSF grant No. 25-22-00762.

[1] R. Weeber et al. (2024), Comprehensive Computational Chemistry, 3, 578-601. [2] C. R. Pike et al., J. Appl. Phys., 1999, 85, 6660

CPP 20.8 Tue 11:30 ZEU/0160

Hydrodynamics substantially affects induced structure formation in magnetic fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Germany

Magnetorheological fluids consist of micrometer-sized magnetic particles suspended in a carrier liquid [1]. Sufficiently strong external magnetic fields lead to the formation of string-like particle aggregates, which results in complex magnetorheological behavior. This mechanism can further be used in the production of magnetic elastomers during the polymerization process when the carrier medium is still fluid and particulate structure formation still possible [2]. Using numerical simulations that spatially resolve both fluid flows and magnetization, we demonstrate that hydrodynamic interactions play a substantial role during structure formation. Hydrodynamics supports the emergence of string-like aggregates, while magnetic interactions align them. Considering besides this fundamental insight the enormous technical importance and potential of magnetic fluids, our results are substantial also from an application perspective.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] S. Odenbach, Arch. Appl. Mech. **86**, 269 (2016).
[2] D. Günther, D. Yu Borin, S. Günther, S. Odenbach, Smart Mater. Struct. **21**, 015005 (2012).

CPP 20.9 Tue 11:45 ZEU/0160

Near-surface colloidal dynamics in jammed and slipping microgel suspensions — •Masoodah Gunny[1], Frédérick Caetano[2], Matilde Bureau[2], Alexandre Vilquin[1], Marie Le Merrer[2], Catherine Barentin[2], and Joshua McGraw[1] — [1]Gulliver - CNRS, ESPCI-PSL 10 Rue Vauquelin 75005 Paris, France — [2]ILM - CNRS, Claude Bernard University, 16 Enrico Fermi 69100 Villeurbanne, France

Jammed suspensions of soft microgel particles exhibit wall slip along smooth boundaries. The direct observation of dynamics within a supposed depletion layer near the wall were difficult to achieve as a result of the layers' supposed sub-micrometric dimensions. We use total internal reflection fluorescence microscopy (TIRFM) to observe colloidal-particle dynamics near the interface between glass and microgel suspensions. Remarkably, microgel suspensions display nanoscale velocity profiles with a slope rupture; particle velocity increases with distance near the wall, and tends to a constant beyond a distance which is characteristic of the ones predicted previously. Beyond velocimetry, we also study the statistical particle altitude distributions near the wall in TIRFM measurements. These distributions are strongly pressure dependent, with nanoparticles more likely found near the solid/liquid interface when the fluid is transported faster near the wall. This high-velocity particle enrichment, not seen for the Newtonian case, is consistent with the development of a depletion layer under such conditions. Taken together, our observations give strong support for the existence of a depletion layer being responsible for wall slip.

CPP 20.10 Tue 12:00 ZEU/0160

Random close packing as a conserved directed percolation transition — •Thomas Axmann and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Soft Matter Theory Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In studying quenches in soft sphere systems O'Hern et al. related the onset of overlaps to isostaticity [1], and consequently to the random close packing scenario. The conditions that lead to the avoidance of overlaps between spheres can be studied with the random organization model [2], which was initially introduced to investigate self organization in sheared colloids. Modifications of this model, which dynamically reduce interparticle overlaps, were used to characterize the random close packing problem as the critical point of a dynamic absorbing state transition in the $d+1$ dimensional conserved directed percolation universality [3,4].

We aim to deepen the understanding of this connection by demonstrating that the configuration change at each time step can be chosen with a fully deterministic strategy while retaining the features of the transition. We clarify difficulties in the treatment of percolating clusters and find that the median overlap depth proves to be a more useful order parameter.

[1] O'Hern et al. PRE 68 (2003)
[2] Corté et al. Nat. Phys. 4 (2008)
[3] Milz et al. PRE 88 (2013)
[4] Wilken et al. PRE 128 (2021)

CPP 20.11 Tue 12:15 ZEU/0160

Rescaled mode-coupling scheme for dynamics in binary mixtures of highly charged colloids — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate dynamic processes in binary mixtures of highly charged colloidal particles by means of Brownian dynamics and multi-component mode-coupling theory (MCT). As input for MCT, thermodynamically consistent, static structure factors from integral equations with Rogers-Young closure are used which are in quantitative agreement to Fourier transforms of static pair correlation functions resulting from simulations.

MCT based on partial structure factors in many-particle systems predicts dynamic properties such as long-time self-diffusion coefficients in qualitative agreement to simulation trajectories. Using instead structure factors from systems with slightly reduced number of effective charges as input, a quantitative agreement of MCT with simulations is achieved. In mixtures of identically charged particles with different short-time mobilities, this rescaled MCT scheme accurately predicts coupling effects in long-time dynamics observed in Brownian dynamics simulations.

CPP 20.12 Tue 12:30 ZEU/0160

Electric double layers - the software package capDFT — Fabienne Dressler and •Andreas Härtel — Institute of Physics, University of Freiburg

Electric Double Layers are used to store electric energy, they can be utilized to harvest energy from waste heat or steps in concentrations, and they stabilize colloidal systems. In all cases, mobile ions arrange themselves to screen surface charges, resulting in sometimes densely packed regions of microscopic particles far from bulk states that dominate the macroscopic physical properties of the system. Modeling these complex systems has theoretical and numerical limitations, but good although expensive solutions exist. We present an open-source software package to treat the described modeling utilizing classical density functional theory [1]. The package has been used successfully in studies of underscreening [2] and allows to go beyond the standard mean-field

approximation of primitive models [3]. We will demonstrate the package by discussing an example, where we study capacities of structured electrodes.

[1] https://github.com/andreashaertel/capdft
[2] Anomalous Underscreening in the Restricted Primitive Model. A. Härtel, M. Bültmann, and F. Coupette. Phys. Rev. Lett. 130, 108202 (2023)
[3] The primitive model in classical density functional theory: beyond the standard mean-field approximation. M. Bültmann and A. Härtel. J. Phys. Condens. Matter 34, 235101 (2022)