

CPP 51: Poster Session III-2

Topics: Active Matter (51.1-51.4), Glasses and Glas Transition (51.5-51.7), Hydrogels and Microgels (51.8-51.14).

Time: Tuesday 14:00–16:00

Location: P2/EG

CPP 51.1 Tue 14:00 P2/EG

Modeling the interaction of magnetically capped colloidal particles — ●MAXIMILIAN NEUMANN¹, ARTUR ERBE², SOFIA S. KANTOROVICH³, PEDRO A. SÁNCHEZ³, SIBYLLE GEMMING^{1,2}, and GABI STEINBACH^{1,2} — ¹Institute of Physics, TU Chemnitz, D-09107 Chemnitz — ²Helmholtz-Zentrum Dresden - Rossendorf, D-01328 Dresden — ³Faculty of Physics, University of Vienna, A-1090 Vienna

Colloidal particles exhibiting spontaneous self-assembly are the precursors to bottom-up fabrication of advanced materials and micromechanical structures. There exists a comprehensive number of different particles with varying types of anisotropy with potential applications for controlled structure engineering. Here, we concentrate on particles that interact via polar fields, which are intrinsically anisotropic. More specifically, we focus on micron-sized silica spheres which are partly covered by a thin ferromagnetic layer with an out-of-plane magnetic anisotropy. With the goal of studying the assembly of such magnetic particles, we introduce a simple two-parameter model: A current-carrying coil enclosed inside a hard sphere is used to approximate an extended magnetization distribution. While the near field induced by the current reflects the extended magnetization, the far field mirrors the stray field of a point dipole. In this model the magnetization distribution is specified by the two coil parameters: The radius and the shift relative to the sphere's center. We present stable assemblies as a function of both parameters.

CPP 51.2 Tue 14:00 P2/EG

The effect of magnetic field and hydrogen peroxide on capped Janus particles — ●YARA ALSAADAWI¹, ANNA EICHLER-VOLF¹, MICHAEL HEIGL², MANFRED ALBRECHT², and ARTUR ERBE¹ — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — ²Institute of Physics, University of Augsburg, Augsburg 86159, Germany

Janus particles are one type of artificial microswimmers consisting of two asymmetrically functionalized surfaces. With proper manipulation, one can control their displacement from one point to another at certain rate, as well as clustering, and orientation. In this work, we prepared Janus particles with caps consisting of Co/Pd, providing magnetic and H₂O₂-catalytic activity for particle propulsion, respectively. To employ both mechanisms, we conducted a systematic work that investigates propulsion under different combination of H₂O₂ concentrations and magnetic fields. Since the magnetic element in the cap plays a critical role in cap orientation and interaction with one another, we studied one particle system as well as two- and three-particle systems. Furthermore, as the swimming behavior is highly affected by the boundary conditions of its surrounding environment, varying surface properties were incorporated during experiments.

CPP 51.3 Tue 14:00 P2/EG

Analytical description of active polar filaments — ●CHRISTIAN ANTON PHILIPPS — Institute for Advanced Simulations, Forschungszentrum Jülich, 52428 Jülich, Germany

Nature provides a variety of active matter agents, which are self-propelled units consume either internal energy or extracting energy from their environment. A particular example on the cellular level are propelled polar semiflexible filaments, e.g., filamentous actin or microtubules in the cell cytoskeleton due to tread-milling and motor proteins [1]. Such active "polymers" exhibit interesting conformational and dynamical properties, even in dilute solution, which are absent in passive systems [2]. From a theoretical point of view, an analytical description of a polar active polymer is rather challenging, specifically due to the directed propulsion by the polar forces. We present an analytical solution of a polar filament with tangential driving forces, where the filament itself is described by the Gaussian semiflexible polymer model [3]. In particular, the inextensibility of the filament is taken into account. In detail, the polymer conformational and dynamical properties emerging by the active force will be discussed. [1] J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. 78, 056601 (2015); [2] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, 101014 (2017); [3] A. Martin-Gomez, T. Eisenstecken, G. Gompper,

R. G. Winkler, Soft Matter 15, 3957 (2019)

CPP 51.4 Tue 14:00 P2/EG

Interplay of surface forces for the directed transport of superparamagnetic beads above a thin film layer substrate — ●KATHARINA GETFERT, RICO HUHNSTOCK, DENNIS HOLZINGER, and ARNO EHRESMANN — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINaT), University of Kassel, Heinrich-Plett-Str. 40, D-34132 Kassel

Directed transport of biofunctionalised magnetic particles over a substrate is a promising mechanism for sensitive analyte detection in lab-on-a-chip devices. Former publications present the realization of controllable superparamagnetic particle transport above a magnetically stripe patterned Exchange-Bias thin film layer substrate, revealing a complex interaction of surface forces between the particles and the substrate [1]. The interplay of these forces determines the steady state distance between both components, which is an important factor for the transport properties. In this work the influence of surface forces on the colloidal stability and, thus, on the particle transport is investigated. The impact on transport properties due to modifications in electrostatic and magnetic interactions between particle and substrate is analyzed by detecting the particle velocity. It can be shown, that the pH-value and thereby the ion-concentration of the surrounding medium plays an essential role in stabilization of the transport system due to its effects on the electrostatic interaction. Furthermore, the increase of the attractive magnetic interaction provides a higher sensitivity in measuring electrolyte dependent transport property changes.

[1] Ehresmann *et al.* (2015), Sensors, 15: 28854-28888.

CPP 51.5 Tue 14:00 P2/EG

Molecular dynamics and ionic conductivity of crown ether based discotics — ARDA YILDIRIM¹, ●MOHAMED AEJAZ KOLMANGADI¹, SABINE LASCHAT², and ANDREAS SCHÖNHALS¹ — ¹Bundesanstalt für Materialforschung und prüfung, Unter den Eichen 87, 12205 Berlin, Germany — ²Institut für Organische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany

In present study, the molecular dynamics of asymmetric crown ether based discotics (KAL) bearing alkyl chains of different lengths were investigated by Broadband Dielectric Spectroscopy (BDS). Three dielectrically active relaxation processes were observed for both materials. At low temperatures, a γ -process in the Cry state was detected and is assigned to the localized fluctuations taking place in the alkyl chains. The $\alpha 1$ -process takes place at higher temperatures in the Colh phase. An $\alpha 3$ process was found in the Colh mesophase. The temperature dependence of the relaxation rates of the $\alpha 3$ process is a completely different than that of the $\alpha 1$ relaxation. Molecular assignments of these different glassy dynamics are proposed. Tgthermal determined by DSC agrees with the dielectric data corresponding to the detected glassy dynamics. In addition, the conductivity contribution of both KAL compounds was analyzed. The conductivity contribution appears in both Cry and Colh phases at temperatures above 300 K.

CPP 51.6 Tue 14:00 P2/EG

Elektrische und mechanische Relaxationsspektroskopie von Säurehydraten — ●SIMON AHLMANN, PHILIPP MÜNZNER, ROLAND BÖHMER and CATALIN GAINARU — Fakultät Physik, Technische Universität Dortmund, 44221 Dortmund

Phosphor- und Schwefelsäure besitzen für viele technische Anwendungen eine große Bedeutung. In wässrigen Lösungen sind diese Säuren durch eine anomal große Leitfähigkeit gekennzeichnet [1]. Es ist jedoch nicht abschließend geklärt, ob diese Leitfähigkeit vor allem auf einen schnellen Protonentransfer oder eher einen Vehikelmehanismus hindeutet, bei dem der Ladungstransport durch die molekulare Bewegung begrenzt wird.

Mittels Rheologie und dielektrischer Spektroskopie haben wir mechanische und elektrische Eigenschaften unterkühlter Phosphorsäure- und Schwefelsäure-Hydrate untersucht. Während die Form der mechanischen Relaxationsspektren des Schwefelsäure-Tetrahydrats temperaturunabhängig ist, gilt dies für Phosphorsäure-Monohydrat nicht.

Dessen thermorheologische Komplexität deuten wir als Konsequenz der ausgeprägten temperaturabhängigen Trennung der mechanischen von den elektrischen Zeitskalen, die wir dielektrisch ermittelt haben [2]. Diese dynamische Entkopplung, die im Schwefelsäure-Hydrat deutlich geringer ausfällt, ist für Anwendungen interessant, die auf einer signifikanten Trennung von Masse- und Ladungstransport beruhen.

[1] M. Heres, Y. Wang, P. J. Griffin, C. Gainaru, A. P. Sokolov, Phys. Rev. Lett. 117, 156001 (2016) [2] M. Frey, H. Didzoleit, C. Gainaru, R. Böhmer, J. Phys. Chem. B 117, 12164 (2013)

CPP 51.7 Tue 14:00 P2/EG

How coupled elementary units determine heterogeneity in macroscopic glass-forming systems — •LAWRENCE SMITH and ANDREAS HEUER — Westfälische Wilhelms-Universität, Münster, Germany

Elementary units of a binary Lennard-Jones glassformer can be identified through quantitative analysis of its underlying potential energy landscape. These units can be fully understood within the continuous time random walk formalism and are found to contain the complete information concerning thermodynamics and diffusivity, while displaying finite size effects with respect to relaxation times and spatial correlations [1]. Previous research has shown that it is possible to identify major contributions to the structural relaxation time τ_α and the non-Gaussian parameter as arising from the moments of the waitingtime distribution for jumps between metabasins of the potential energy landscape [2].

We investigate the impact of a coupling between elementary units on the non-Gaussian parameter (NGP) and τ_α to establish a relationship between this coupling and finite size effects that can be observed in molecular dynamic simulations. We extend this idea to gain insight into mechanisms underlying the emergence of dynamic heterogeneity as measured by four-point correlation functions in the stochastic model as well as in molecular dynamics simulations.

[1] C. Rehwald, A. Heuer, Phys. Rev. E 86, 051504 (2012)

[2] C. Schroer, A. Heuer, Phys. Rev. Lett. 110, 067801 (2013)

CPP 51.8 Tue 14:00 P2/EG

Co-nonsolvency transition of PNIPMAM-based block copolymer thin films in a series of binary mixtures — •PEIXI WANG¹, CHRISTINA GEIGER¹, LUCAS P. KREUZER¹, TOBIAS WIDMANN¹, ROBERT CUBITT², ANDRÉ LASCHEWSKY³, CHRISTINE M. PAPADAKIS⁴, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Institut Laue-Langevin, 38042 Grenoble, France — ³Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany — ⁴TU München, Physik-Department, Physik weicher Materie, 85748 Garching

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich phase in a certain range of compositions of these two solvents. The nonionic thermo-responsive polymer, poly(isopropylmethacrylamide) (PNIPMAM), which features a lower critical solution temperature (LCST) in aqueous solution, has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethylammonio)butane-1-sulfonate)) (PSBP)*which exhibits an lower upper critical solution temperature (UCST) and shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPAM thin films in a series of deuterated binary mixtures by using time-of-flight neutron reflectometry (TOF-NR).

CPP 51.9 Tue 14:00 P2/EG

Hydrodynamics and Response of PNIPAM Microgel Aqueous Solution Subjected to Acoustic Waves — •AMIN RAHIMZADEH and REGINE VON KLITZING — Physics department, Technical University of Darmstadt, Germany

The poly(N-isopropylacrylamide)(PNIPAM) stimuli-responsive microgels were the subject of studies so far where their reaction to changes in temperature in aqueous solutions has been systematically investigated. Microgels shrink in the solution above their volume phase transition temperature(VPTT) due to the breaking of hydrogen bonds between PNIPAM and the solvent. Acoustic waves, on the other hand, can transfer a certain amount of energy by penetrating into a liquid solution. Depending on the wave frequency and amplitude, flow patterns inside of the liquid affected by the propagating waves can result in

microstreaming to atomization and micro drop ejection. We transfer acoustic waves into a sessile water droplet containing PNIPAM microgels to study their response by carefully tuning the ultrasonic power. Therefore, the amount of energy enough for breaking the hydrogen bonds-that is not high to deteriorate the polymer chains-is a crucial parameter in this context. The shrinking/swelling behavior, dynamic stiffness, as well as streaming pattern of microgels, are subjected to analyze in this work.

CPP 51.10 Tue 14:00 P2/EG

PNIPAM microgels at the air-water interface - Influence of cross-linking concentration and distribution — •FRANZISKA JAKOB, MATTHIAS KÜHNHAMMER, and REGINE VON KLITZING — Technical University of Darmstadt, Department of Physics, Soft Matter at Interfaces, 64287 Darmstadt, Germany

Poly-N-isopropylacrylamide (PNIPAM) is a deformable and temperature-responsive polymer microgel, which can adsorb at liquid interfaces. It has been in the focus of multitudinous studies in the past years and is still being discussed very actively in the context of various possible applications, because of their ability to respond to external stimuli like temperature.

Spreading of microgels at the air-water interface depends considerably on various parameters. One important factor is the cross-linking density that has a strong influence on the microgel film formed at the air-water interface, and thus a significant impact on the compression isotherm¹.

In this contribution, films prepared from microgels with different cross-linking concentrations and different cross-linking distributions are studied. From this, conclusions regarding the degree of interdigitation (transition from core-core to shell-shell contact) of different microgels are drawn.

[1] C. Picard et al. Organization of Microgels at the Air-Water Interface under Compression: Role of Electrostatics and Cross-Linking Density. *Langmuir* **2017**, p.7973 f.

CPP 51.11 Tue 14:00 P2/EG

Magnetic nanogels in the flow — •IVAN NOVIKAU¹, EKATERINA NOVAR², PEDRO SANCHEZ², and SOFIA KANTOROVICH^{1,2} — ¹University of Vienna — ²Ural Federal University

Nanogels (NGs) with multifunctionalized magnetic nanoparticles (MNPs) have demonstrated the ability to effectively destroy cancer cells in vivo, without causing visible damage to healthy organs [1].

The presence of MNPs inside the NGs also offers an additional mechanism to control their properties by means of applied magnetic fields.

Our study of a suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel, and the self-assembly in the given system, strongly depend on the strength of dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a shear flow by means of molecular dynamics computer simulations coupled with Lattice-Boltzmann algorithm. Each NG is initially modeled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. MNPs are randomly incorporated into this network [3].

Dipolar coupling, shear rate and viscosity of the carrier liquid are used as control parameters to alter both self-assembly of NGs and individual structural properties.

[1] Qing Wu et al., Nat. Commun., 10 (240), 2019.

[2] Novikau et al., JMMM, 2020.

<https://doi.org/10.1016/j.jmmm.2019.166152>

[3] Minina et al., J. Mol. Liq., 289, 2019.

CPP 51.12 Tue 14:00 P2/EG

Design and characterization of hydrogel bilayer strips with different crosslink densities — •JONAS STAUDENMEIR¹, LUKAS CONRADS¹, SEBASTIAN MEYER¹, NIKLAS O. JUNKER¹, DMITRY N. CHIGRIN^{1,2}, and GERO VON PLESSSEN¹ — ¹Institute of Physics (IA), RWTH Aachen, Germany — ²DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Hydrogels are three-dimensional structures made of cross-linked polymers that can absorb and store large amounts of solvents. By changing external parameters (temperature, pH, etc.) hydrogels react with large volume changes by ejecting or absorbing the solvent. Due to such volume changes, bilayers consisting of a hydrogel and a passive elastic material are known to show bending upon temperature changes. To develop a bistable system, which performs a snap-through transition between low- and high temperature states, hydrogel bilayer strips

consisting of two poly(*N*-isopropylacrylamide) (PNIPAm) layers with different crosslinker density were designed and investigated in a water bath. Due to the different swelling properties of the layers, the strips showed a curvature that could be continuously changed by slow heating and cooling. By fixing the strip ends to a flexible polydimethylsiloxane (PDMS) frame, a sudden change in the direction of curvature was observed upon heating. Experimental and simulation results are compared.

CPP 51.13 Tue 14:00 P2/EG

Investigation of Non-Equilibrium Bending Dynamics of Microgel Disks — •NIKLAS O. JUNKER¹, FELIX JIANG¹, OLIVER JUNG², SEBASTIAN MEYER¹, DMITRY N. CHIGRIN^{1,2}, AHMED MOURRAN², MARTIN MÖLLER², and GERO VON PLESSEN¹ — ¹Institute of Physics (IA), RWTH Aachen, Germany — ²DWI - Leibniz Institute for Interactive Materials, Aachen, Germany

Microgels are cross-linked polymer networks of micrometer or submicrometer dimensions which, in a solvent, can undergo large and fast volume changes in response to variations of external parameters (temperature, pH, etc.). Due to such volume changes, bilayers consisting of a hydrogel and a passive elastic material are known to show bending behavior. In the present work, bilayer disks of elliptical shape and consisting of a gold-nanorod-loaded, 5 micrometer thick poly(*N*-isopropylacrylamide) (PNIPAm) layer and a gold nanolayer are investigated in water. Non-equilibrium actuation dynamics triggered

by conventional and photothermal heating is observed. The microgel structures are found to bend differently upon conventional temperature changes than upon photothermal heating. This behavior is systematically studied for different heating rates (up to 20°C/min for conventional heating and up to 1°C/ms for photothermal heating, in which the gold nanorods are used as photoabsorbers and local heaters).

CPP 51.14 Tue 14:00 P2/EG

Bending Simulations of Hydrogel Bi-layer Beams — •SEBASTIAN MEYER¹, LUKAS CONRADS¹, JONAS STAUDENMEIR¹, TOBIAS ABEL¹, NIKLAS JUNKER¹, GERO VON PLESSEN¹, and DMITRY CHIGRIN^{1,2} — ¹Institute of Physics (IA), RWTH Aachen, Germany — ²DWI Leibniz Institute for Interactive Materials, Aachen, Germany

Hydrogels are cross-linked polymer networks that exhibit a great capacity to absorb and store large amounts of solvent. The amount of solvent in the hydrogel depends strongly on external parameters like the temperature, pH-value, etc., of the surroundings. Therefore, variations of these parameters can lead to large volume changes of the hydrogel. Two connected layers of differently cross-linked gels will start to bend, with the bending curvature depending on the temperature of the surroundings. Here, we present a theoretical description of such a bending for free and constrained hydrogel bi-layer beams using both classical beam theory and 3D finite volume simulations. Further, we compare the results to experimental observations.