DY 43: Soft Matter

Time: Friday 10:15–12:30 Location: ZEU 118

DY 43.1 Fri 10:15 ZEU 118

Mobility and Diffusion of a Tagged Particle in a Driven Colloidal Suspension — •Boris Lander[1], Udo Seifert[1], and Thomas Speck[2,3] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [2]Department of Chemistry, University of California, Berkeley, California 94720, USA — [3]Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Mobility and diffusion of single particles play a key role in the understanding of colloidal suspensions. While beyond linear response, diffusion coefficients can still be obtained by a Green-Kubo relation, determining the mobility is challenging. A novel method enables us to compute the time-dependent response function for a single tagged particle perturbed by a small force and thus the mobility in a Brownian dynamics simulation [1]. For a suspension driven into a nonequilibrium steady state by simple shear flow, both mobility and diffusion constant of the tagged particle increase with shear. Our data can be approximated by an expansion, where the mobility becomes proportional to the square root of the strain rate. Somewhat surprisingly, the initial decay of the velocity autocorrelation function can be mapped onto a corresponding response function by a time-independent scaling factor, allowing for an interpretation in terms of an 'effective temperature'. Such a phenomenological effective temperature recovers the Einstein relation in nonequilibrium.

[1] B. Lander, U. Seifert, T. Speck, EPL, in press.

DY 43.2 Fri 10:30 ZEU 118

Entanglements in globular polymer phases: A Monte Carlo study — •Daniel Reith and Peter Virnau — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55099 Mainz

Bridging algorithms are global Monte Carlo moves which allow for simulation of globular phases of single polymers [1]. These moves ensure an efficient sampling of the topological degrees of freedom, which is usually hindered by the high monomer density and self-entanglements, by destroying and recreating bonds. In this context, the determination of knots provides a measure for entanglement which allows us to gauge the efficiency of the move sets.

The second part will focus on the application of these bridging moves to problems related to single chain polymers in globular phases. To this end we discuss single polystyrene chains in miniemulsion droplets, the influence of chain stiffness on self-entanglements of a single polymer chain in a spherical capsid and the influence of sequence on the knotting of globular heteropolymers.

[1] D. Reith, P. Virnau, Comput Phys Commun **181**, 800 (2010)

DY 43.3 Fri 10:45 ZEU 118

Friction controlled bending solitons as folding pathway toward colloidal clusters — •Nebojsa Casic[1], Steffen Schreiber[2], Pietro Tierno[3], Walter Zimmermann[2], and Thomas M. Fischer[1] — [1]EP V, Uni Bayreuth, Germany — [2]TP 1, Uni Bayreuth, Germany — [3]Departament de Química Física, Universitat de Barcelona, Spain

We study the conformational transition of an ensemble of magnetic particles from a linear chain to a compact cluster when subjected to an external magnetic field modulation. We show that the transient dynamics induced by switching the field from static to rotating is governed by the relative friction of adjacent particles in the chain. Solid particles show bending solitons counter-propagating along the chain while buckling of the chain is the mechanism preferred by ferrofluid droplets. By combining real-space experiments with numerical simulations we unveil the underlying mechanism of folding pathways in driven colloidal systems. EPL, 90 (2010) 58001

DY 43.4 Fri 11:00 ZEU 118

Switching A Gelified Liquid Crystal — •Thomas Müller[1], Maxim Khazimullin[2], Ingo Rehberg[1], Wolfgang Schöpf[1], Alexei Krekhov[3], Robin Pettau[4], and Klaus Kreger[4] — [1]Experimental Physics V, University of Bayreuth, 95440 Bayreuth, Germany — [2]Institute of Molecule and Crystal Physics, Russian Academy of Science, Ufa, Russia — [3]Theoretical Physics I, University of Bayreuth, 95440 Bayreuth, Germany — [4]Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Liquid crystal displays make use of the electrooptical effect, caused by the orientation of the liquid crystals in an external electrical field above a certain threshold voltage (Fréedericksz effect). We investigate this effect in a new class of liquid crystal material, namely a diluted solution of an ABA-triblock copolymer in the nematic liquid crystal 5CB. The motivation of our studies is to obtain the physical parameters of this novel material with special emphasis on its dynamical behavior. In our experiments we use polarizing microscopy to detect the electrically controlled birefringence in homogeneous cells. We measure the temporal evolution of the light intensity when switching the electrical field above and below the threshold. It provides information about relaxation times of the director orientation, which can be used to determine the Fréedericksz threshold voltage and the elasticity of the gelified liquid crystal. Moreover, the relaxation times yield the rotational viscosity which contains information about the interaction between polymer molecules and liquid crystals.

DY 43.5 Fri 11:15 ZEU 118

Phase diagram and orientational dynamics of nematic liquid crystals under shear flow: A numerical bifurcation analysis. — •David A. Strehober and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study the nonequilibrium dynamics of rodlike nematic polymers under shear flow. Starting from a mesoscopic description involving the alignment tensor [1][2], we investigate the rheological phase diagram with respect to the shear rate and tumbling parameter. The dynamics of the alignment tensor is described by five coupled differential equations. We employ numerical continuation methods, specifically the freely available software package MATCONT [3], to find the boundaries between different dynamic states. We recover the results that were obtained via direct integration [4] of the set of differential equations for the alignment tensor. On top of that, we are able to make statements about the nature of the bifurcations, and how orientational modes, i.e. Kayaking Wagging or Tumbling, are born. We conclude the talk with a discussion of the role of temperature.

[1] S. Hess, Z.Naturforsch. A **31a**, 1034 (1976)
[2] M. Doi, J.Polym. Sci., Polym. Phys. Ed. **19**, 229 (1981)
[3] A. Dhooge, W. Govaerts, and Yu. A. Kuznetsov., ACM Trans. Math. Softw. **29**, (2003)
[4] S. Grandner, S. Heidenreich, S. Hess and S. H. L. Klapp, Eur.Phys.J. E **24**, 353 (2007)

DY 43.6 Fri 11:30 ZEU 118

Helical crystals of charged colloids in cylindrical confinement — •Erdal Celal Oguz, René Messina, and Harmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

By lattice sum calculations we explore the ground state phase diagram of screened Coulomb particles in a cylindrical confinement. We obtain several chiral as well as achiral helical phases. Similar systems were studied with dusty plasmas [1] and hard spheres [2]. We also compare our results to computer simulations and experiments with highly screened particles [2,3].

[1] V. N. Tsytovich, G. E. Morfill, V. E. Fortov, N. G. Gusein-Zade, B. A. Klumov and S. V. Vladimirov, New Journal of Physics **9**, 2007
[2] G. T. Pickett, M. Gross and H. Okuyama, Phys. Rev. Lett. **85**, 2000
[3] M. Tymczenko, L. F. Marsal, T. Trifonov, I. Rodriguez, F. Ramiro-Manzano, J. Pallares, A. Rodriguez, R. Alcubilla and F. Meseguer, Adv. Mater. **20**, 2008

DY 43.7 Fri 11:45 ZEU 118

Binary non-additive hard sphere mixtures: Fluid demixing, asymptotic decay of correlations and free fluid interfaces — •Matthias Schmidt[1,2] and Paul Hopkins[2] — [1]Theoretische Physik II, Physikalisches Institut, Universität Bayreuth, D-95440 Bayreuth, Germany — [2]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

Using a fundamental measure density functional theory we investigate both bulk and inhomogeneous systems of the binary non-additive hard

sphere model. For sufficiently large (positive) non-additivity the mixture phase separates into two fluid phases with different compositions. We calculate bulk fluid-fluid coexistence curves for a range of size ratios and non-additivity parameters and find that they compare well to simulation results from the literature. Using the Ornstein-Zernike equation, we investigate the asymptotic decay of the partial pair correlation functions. At low densities a structural crossover occurs in the asymptotic decay between two different damped oscillatory modes with different wavelengths corresponding to the two intra-species hard-core diameters. On approaching the fluid-fluid critical point there is a Fisher-Widom crossover from exponentially damped oscillatory to monotonic asymptotic decay. Using the density functional we calculate the density profiles for the planar free fluid-fluid interface between coexisting fluid phases. We show that the type of asymptotic decay of the pair correlation functions not only determines the asymptotic decay of the interface profiles, but is also relevant for intermediate and even short-ranged behaviour.

DY 43.8 Fri 12:00 ZEU 118

Conformational studies of bottle-brush polymers absorbed on a flat solid surface under good solvent conditions — •Hsiao-Ping Hsu[1], Wolfgang Paul[2], and Kurt Binder[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Theoretische Physik, Martin Luther Universität Halle-Wittenberg, Halle, Germany

The adsorption of a bottle-brush polymer end-grafted with one chain end of its backbone to a flat substrate surface is studied extensively by Monte Carlo simulations. The bond fluctuation model on the simple cubic lattice, is used here [1]. Varying the backbone chain length and the side chain length, and fixing the grafting density to 1, our simulations cover the range which is accessible for the comparison of experimental data and the theoretically scaling predictions. When the adsorption energy strength is varied, we find that the adsorption transition roughly occurs at the same value as for ordinary linear chains. For longer side chains we show that the adsorption of bottle-brushes is a two step process, the decrease of the perpendicular linear dimension of side chains with adsorption energy strength can even be non-monotonic [2]. As the bottle-brush polymer is deeply adsorbed to the surface, the evidence for a quasi-two-dimensional scaling is presented.

[1] H.-P. Hsu, W. Paul, and K. Binder, Macromolecules **43**, 3094 (2010).

[2] H.-P. Hsu, W. Paul, and K. Binder, J. Chem. Phys. **133**, 134902 (2010)

DY 43.9 Fri 12:15 ZEU 118

Quantum-classical adaptive simulation of liquid para-hydrogen — •Adolfo Poma and Luigi Delle Site — Max-Planck-Institute for Polymer Research, Ackermannweg 10, D-55021 Mainz, Germany

Adaptive resolution simulations for classical systems are currently made within a reasonably consistent theoretical framework. Recently we have extended this approach to the quantum-classical coupling by mapping the quantum nature of an atom onto a classical polymer ring representation within the path integral approach. In this way the process of interfacing adaptively a quantum representation to a classical one corresponds to problem of interfacing two regions with a different number of effective "classical" degrees of freedom; thus the classical formulation of the adaptive algorithm applies straightforwardly to the quantum-classical problem. In this work we show the robustness of such an approach for a liquid of para-hydrogen at low temperature. This system represents a highly challenging conceptual and technical test for the adaptive approach due to the extreme thermodynamical conditions where quantum effects play a central role.