CPP 44: Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 2

organized by Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TUM) and Walter Richtering (RWTH Aachen)

Time: Friday 9:30–11:15 Location: H38

Invited Talk CPP 44.1 Fri 9:30 H38

Connecting dynamics and phase behavior of proteins: The neutron perspective — •Frank Schreiber — Universität Tübingen, Germany

We discuss the combination of various neutron scattering techniques to shed light on the dynamics of proteins in aqueous solution. This includes several processes, such as backbone and side-chain fluctuations, interdomain motions, as well as global rotational and translational (i.e. center of mass) diffusion. Since protein dynamics is related to protein function and essential transport processes, a detailed mechanistic understanding and monitoring of protein dynamics in solution is highly desirable. In particular, we connect it to the overall phase behavior in terms of clustering, crowding, crystallization, and phase separation [1], employing a combination of elastic, quasi-elastic, and inelastic scattering [2] as well as complementary techniques, such as X-ray photon correlation spectroscopy (XPCS) and simulations [3]. Finally, we comment on future perspectives with advanced neutron sources. Invaluable contributions by numerous collaborators are gratefully acknowledged.

[1] M. Grimaldo et al., JPCL, 10, 1709 (2019) [2] M. Grimaldo et al., Quarterly Reviews of Biophysics, 52, e7 (2019) [3] A. Girelli et al., Phys. Rev. Lett. 126 (2021) 138004

CPP 44.2 Fri 10:00 H38

Self-assembly of supramolecular magnetic polymers with monomers of different sizes — Ekaterina Novak[1], Elena Pyanzina[1], •Marina Gupalo[1], and Sofia Kantorovich[1,2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

In this paper we studying the effect of polydispersity of magnetic particles on the self-assembly of supramolecular magnetic polymers. Magnetic polymers are widely used to create new magnetically controlled materials and represent an analogue of polymer chains, where polymer molecules serve as crosslinks, and magnetic particles replace monomers. We propose to consider the bidisperse model, which takes into account only two fractions of particles in size, which is enough to track the main influence of polydispersity on the self-organization of a magnetic polymer. Using the method of computer simulation of Langevin's dynamics, we study various structural parameters of an individual magnetic polymer of different configurations: a chain, a closed ring, an X-shaped and Y-shaped magnetic filament. For analysis of the qualitative changes in equilibrium properties with temperature were used radius of gyration and magnetic moment, the general microstates are also defined. It turned out that the considered new types of polymer configuration compared with the monodisperse model significantly affect the equilibrium properties. This work was supported by RSF grant 19-72-10033.

CPP 44.3 Fri 10:15 H38

Pathways of micellar collapse and swelling of PMMA-*b*-PNIPAM in aqueous solution after a rapid change of pressure — •Pablo A. Alvarez Herrera[1], Johannes Allwang[1], Feifei Zheng[1], Cristiane Henschel[2], Leonardo Chiappisi[3], Alfons Schulte[4], André Laschewsky[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut für Chemie, Potsdam-Golm, Germany — [3]Institut Laue- Langevin, Grenoble, France — [4]University of Central Florida, Orlando, USA

In aqueous solution, diblock copolymers consisting of a permanently hydrophobic and a thermo-responsive block can self-assemble into different morphologies. In particular, poly (methyl methacrylate)-*b*-poly(*N*-isopropylacrylamide) (PMMA-*b*-PNIPAM) forms spherical micelles featuring a PMMA core and a thermo-responsive PNIPAM shell. At atmospheric pressure, the micellar shell dehydrates, and the collapsed micelles form aggregates when heating above the cloud point of PNIPAM [1]. This phase transition can be also induced by changing the pressure. In this contribution, we study the micellar collapse and their posterior aggregation by kinetic small-angle neutron scattering (SANS) in combination with rapid pressure jumps across the co-existence line. The disintegration of the aggregates and the micellar swelling are also investigated by performing the pressure jump in the opposite direction.

[1] C.-H. Ko, C. M. Papadakis et al., Macromolecules 54, 384 (2021).

CPP 44.4 Fri 10:30 H38

Investigation of the Effect of Magnesium Salts with Chaotropic Anions on the Swelling Behavior of PNIPMAM Thin Films — •Julija Reitenbach[1], Christina Geiger[1], Peixi Wang[1], Robert Cubitt[2], Dirk Schanzenbach[3], André Laschewsky[3], Christine M. Papadakis[4], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

Thermoresponsive polymer thin films have gained a lot of attention in the past decades due to their attractiveness for a wide range of applications. A variety of polymer showing LCST- or UCST-type behavior are known, and their transition temperatures can be influenced by various factors such as molar mass, end groups, copolymerization, or by the addition of salts. For polymers in aqueous solution, it was found that the folding of the polymer chains can be strongly influenced by the type of salt and this ability follows a trend called the Hofmeister series. While this effect is well known in solution, the influence on the swelling behavior of PNIPMAM thin films has yet to be investigated thoroughly. We aim to elucidate the underlying mechanism by spectral reflectance and time-of-flight neutron reflectometry on a macroscopic scale and by in situ Fourier-transform infrared spectroscopy on a molecular level.

Invited Talk CPP 44.5 Fri 10:45 H38

Magnetic particle self-assembly at functionalized interfaces — •Max Wolff — Department for Physics and Astronomy, Uppsala University, Uppsala, Sweden

Neutrons allow the study of buried interfaces and are directly sensitive to magnetic induction. This makes grazing incidence neutron scattering an ideal tool for the study of self-assembled magnetic particles.

In this talk I will discuss the self-assembly of monodisperse colloidal magnetite nanoparticles from a dilute water-based ferrofluid onto functionalized silicon surfaces. The density of the layer adjacent to the substrate is determined by the interaction between the particles and the substrate. Dense layers form for chemical binding and magnetic substrates, while less dense and no layering is found for physisorption and repulsive interactions. Once adsorbed subsequent layers assemble due to magnetic dipolar forces. The layering gets more pronounced for larger dipole moments of the particles. Once formed the density and structure of the layers may be tuned by magnetic and/or shear fields.

Magnetic particles may also be used to self-assemble polymer micelles. Applied magnetic fields may result in a micro shear effect aligning the domains of micellar crystals. By stroboscopic reintegration this reorientation process may be followed on time scales down to ms and resonant enhancement may aid the identification of off-specular and grazing incidence small angle scattering.