CPP 42: French-German Session: Nanomaterials, Composites and Hybrids II

Time: Wednesday 17:00–18:45 Location: ZEU/0260

Invited Talk CPP 42.1 Wed 17:00 ZEU/0260

Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS — •Julian Oberdisse and Anne-Caroline Genix — Laboratoire Charles Coulomb, U Montpellier France

Understanding the molecular structure of mesoporous solid ionic systems is crucial for optimizing macroscopic properties, in particular ionic transport for energy applications, as well as mechanical flexibility. These systems can be synthesized efficiently under "one-pot" conditions, which rely on mesopore formation through microphase separation of templating ionic liquids.

In the present study, the phase transitions of the embedded ionic liquid have been studied by wide-angle scattering, QENS, DSC, and BDS, as a function of confinement. Then, poly(ionic liquid)s have been added in order to incorporate both connectivity and modify mechanical strength. We report on the structural analysis of ionic liquid and poly(ionic liquid) embedded in ionosilica matrices, employing a combination of small-angle scattering of neutrons and X-rays, isotopic substitution, and physico-chemical solvent-based extraction methods. Data analysis is based on molecular modelling with an original, quantitative comparison of the scattering curves under different contrasts. In agreement with NMR, it is shown that these mesoporous systems have an unexpected molecular structure, with the ionic liquid counterions penetrating the ionosilica matrix surrounding the mesopores. The poly(ionic liquid) forms patches decorating the pore walls, with tunable conformation sensitive to solvent conditions.

CPP 42.2 Wed 17:30 ZEU/0260

Plasmonic core-shell microgels: The role of the core size — •Déborah Feller[1,2], Julian Oberdisse[3], Sylvain Prévost[4], and Matthias Karg[1] — [1]Physical Chemistry of Functional Polymers, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Physical Chemistry: Colloids and Nanooptics, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [3]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, Montpellier, France — [4]Large Scale Structures, Institut Laue-Langevin, Grenoble, France

Gold-poly-N-isopropylacrylamide (Au PNIPAM) core-shell microgels are interesting due to the localized surface plasmon resonance (LSPR) of the cores. The LSPR position strongly depends on the core size. Compared to other core-shell microgels, Au cores can be precisely overgrown in the shell in situ. Although cores grow in size, the overall hydrodynamic diameter of the microgels does not change. It is not known how the structure of the shell changes during the overgrowth.

Here, we are analyzing Au-PNIPAM microgels with two crosslinker densities. The cores are overgrown from 14 nm in diameter to nearly 100 nm. We perform small-angle X-ray and neutron scattering (SAXS/SANS) to study the respective form factors. SAXS provides information about the cores and SANS about the shell. We also investigate temperature-dependent changes in the microgel by SANS. Additionally, extinction spectra are recorded to study the optical properties. We perform simulations of the different microgels to get information on the internal structure of the shell and the polymer distribution.

CPP 42.3 Wed 17:45 ZEU/0260

Consequences of the near-field effect in highly filled magneto-active elastomers — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden

In many theoretical models for magneto-active elastomers (MAEs) the interactions among magnetic/magnetizable particles are approximated via dipole models. In highly filled samples, as well as in structured MAEs, the particles are often very close to each other. In such situation the dipole approximation largely underestimates the interactions among magnetizable particles. Yet, for only 2 spherical particles the analytic solution is quite complex, resulting in a slowly converging series expansion. When considering many particle systems only computationally elaborate methods like a finite element approach can provide numerical solutions. Based on a compact fitting function for the 2-body problem, we suggest an accurate approximation for many-body systems including the near-field effect beyond dipole interactions. Considering these corrections due to the near-field effect in comparison to the dipole approximation, we further investigate the role of cluster formation and dispersion of particles in MAEs when an external magnetic field is applied or switched off.

CPP 42.4 Wed 18:00 ZEU/0260

Magneto-active elastomers with magnetically hard vs soft particles: molecular dynamics simulations — •Júlio P. A. Santos and Sofia Kantorovich — University of Vienna, Faculty of Physics, Kolingasse 14-16, 1090 Vienna, Austria

Magneto-active elastomers (MAEs) [1-2], or magnetorheological elastomers (MREs), are composite materials whose properties - such as stiffness, surface roughness (wettability), and shape - can be controlled by low-energy magnetic fields, making them ideal for soft robotics. MAEs consist of an elastic matrix embedded with magnetic micro- or nanoparticles, magnetically either hard (MH) or soft (MS). For high concentrations of MH particles, one can use a complex arrangement of springs that randomly bond nearby MH particles [3]. However, this model oversimplifies particle behavior (as permanent point dipoles) - critical for modeling physically relevant MAEs.

We address these issues in ESPResSo [4], employing molecular dynamics to study the impact of MS particles on the surface relief of a MAE layer and to provide a critical comparison between MH- and MS-based MAEs. At zero field, MS particles do not interact magnetically, whereas MH particles form long chains within the layer. Increasing the field slowly promotes dipolar interactions between the MS particles and rapidly promotes Zeeman interactions with the applied field, leading to chains that preferentially align parallel to it. In contrast, MH chains must break before reorienting in the direction of the magnetic field, due to the greater importance of dipolar interactions relative to Zeeman, requiring larger applied fields for signficant surface structural changes.

CPP 42.5 Wed 18:15 ZEU/0260

Microstructure analysis of intermediate states in the structure formation process of magnetorheological elastomers — •Nils Magin and Stefan Odenbach — TU Dresden

A composite of magnetic particles and an elastic polymer matrix is referred to as a magnetorheological elastomer. The size and concentration of magnetic particles, as well as the elasticity of the matrix, are the determining factors in the magnetorheological (MR) effect of such materials. Materials exhibiting significant MR properties are commonly referred to as MR elastomers. The application of an external homogeneous magnetic field during the polymerisation process enables the structuring of particles in the initially liquid polymer matrix, resulting in the fabrication of an anisotropic (or structured) material. In order to facilitate a more profound comprehension of the structural formation, the application of the magnetic field is initiated at discrete phases of the polymerisation process. This process gives rise to intermediate states in the structuring that can be observed. The microstructure is examined using computer X-ray tomography and image processing. Furthermore, the influence of the magnetic field, particle concentration, and sample height on the microstructure is discussed. We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 42.6 Wed 18:30 ZEU/0260

Approximate doubling of the magnitude of maximized magnetorheological effects — Lukas Fischer[1,2] and •Andreas M. Menzel[1] — [1]Otto von Guericke University Magdeburg, Magdeburg, Germany — [2]The University of Osaka, Osaka, Japan

In its static limit, the magnetorheological effect of magnetic elastomers implies changes of elastic moduli by external magnetic fields. Induced magnetic interactions between magnetizable inclusions in a soft, elastic, polymeric matrix affect the overall mechanical stiffness.

First, we optimized the spatial arrangement of the magnetizable inclusions to achieve the strongest change in overall elastic moduli, either for maximized overall stiffening or softening [1]. We focused on both, Young and shear moduli.

Second, in combination, we simultaneously optimized the structural organization to achieve maximized stiffening when an external magnetic field is applied in one direction, but maximized softening when the field is applied along a perpendicular direction [2]. In our case, switching between these two field directions can approximately double the magnitude in overall change of elastic moduli.

Once experimental realizations of prescribed structuring become

possible, our strategy provides a direct route to further extend the potential of the materials.

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

[1] L. Fischer, A. M. Menzel, PNAS Nexus **3**, pgae353 (2024).
[2] L. Fischer, A. M. Menzel, arXiv:2507.22777 (2025).