

CPP 1: Focus: Morphology of Complex Polymer Mesophases: From Experiment to Modelling - organized by Kostas Daoulas and Volker Abetz

Time: Monday 9:30–12:30

Location: H14

Invited Talk CPP 1.1 Mon 9:30 H14
Building Complex Colloids with Block Copolymers and Topology — ●ANDRE GROESCHEL — Physical Chemistry and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg Essen, 47057 Duisburg, Germany

Colloids are omnipresent in nature as well as our everyday lives, e.g. in paint, milk, as quantum dots or colloidal gold. For technological applications colloids are typically synthesized using equipment or wet chemical processes giving access to particles of well-controlled sizes. In nature however, biological colloids are often self-assembled from smaller building blocks. Virus particles are composed of a defined number of proteins, giving viruses a complex composition, surface chemistry, and in some cases, also shape-anisotropy on length scales as small as 20 nm. Inspired by the natural structuring abilities, self-assembly concepts are now researched that allow the synthesis of colloids with comparable level of detail and control.

This presentation summarizes our efforts to create complex colloids using concepts of self-assembly, block copolymers and topology. Block copolymers are comparably primitive but versatile building blocks that are able to assemble into microparticles with unusual shapes, mesoscopic inner structure, and functional 2D/3D surfaces. To better understand the relationship between topology an mesostructure, we analyze the particles with electron tomography and resolve the delicate 3D arrangement of polymer domains through reconstructions.

Invited Talk CPP 1.2 Mon 10:00 H14
Gradient dynamics models for films of complex fluids and beyond - Dewetting, line deposition and crystallisation — ●UWE THIELE — Institut für Theoretische Physik and Center for Nonlinear Science, Universität Münster.

First, we review situations where the dynamics of phase transitions creates structures, e.g., dewetting polymer mixtures, Langmuir-Blodgett (LB) transfer of surfactants or colloidal crystallisation. After presenting typical hydrodynamic thin-film models we rewrite them as gradient dynamics on some energy functional that accounts for wettability and capillarity. This allows for many consistent extensions, e.g., towards solute-dependent wettability. As example we show that a film of a mixture may become unstable through coupled film height and concentration fluctuations. Next, we consider gradient dynamics models for films covered by surfactants. Such models may be employed to describe the formation of line patterns during LB transfer of a surfactant layer from a bath onto a moving plate. After showing simulations with the full model, we sketch how line deposition is reflected in an intricate bifurcation structure that one can analyse within a Cahn-Hilliard-type model. Finally, we consider colloidal crystallisation employing gradient dynamics models, namely, dynamical density functional theory (DDFT) and its local approximation, the phase field crystal (PFC) model. We analyse crystallisation fronts and show that their speeds may be obtained via a marginal stability criterion and relate it to created disorder and subsequent aging. Finally, we discuss the relation of localised states and an amorphous solid phase.

CPP 1.3 Mon 10:30 H14
Optimum Disorder of Polymer Mesoparticle Aggregates for Efficient Thermal Insulation — FABIAN NUTZ¹, ALEXANDRA PHILIPP¹, BERND KOPERA¹, MARTIN DULLE², and ●MARKUS RETSCH¹ — ¹Physical Chemistry I, University of Bayreuth, 95447 Bayreuth, Germany — ²JCMS-1/ICS-1: Neutron Scattering Forschungszentrum, Juelich, Germany

Heat transport plays a critical role in modern batteries, electrodes, and capacitors. This is caused by the ongoing miniaturization of such nano-technological devices, which increases the local power density and hence temperature. Even worse, the introduction of heterostructures and interfaces is often accompanied by a reduction in thermal conductivity, which can ultimately lead to the failure of the entire device. Surprisingly, a fundamental understanding of the governing heat transport processes even in simple systems is still missing. This contribution closes this gap and elucidates how strongly the morphology of a model particulate system influences the effective thermal conductivity across such a complex mesostructure. In a combined experimental and modeling approach, well-defined mixtures of monodisperse parti-

cles with varying size ratios were investigated. The transition from order to disorder can reduce the effective thermal conductivity by as much as ~50%. This is caused by an increase in the thermal transport path length and is governed by the number of inter-particle contact points.

Invited Talk CPP 1.4 Mon 10:45 H14
Controlling structure, orientation and nanomorphology in semi-conducting and conducting polymer films — ●MARTIN BRINKMANN, LAURE BINIEK, VISHNU VIJAYAKUMAR, and VIKTORIIA UNTILOVA — Université de Strasbourg, Institut Charles Sadron, CNRS, Strasbourg, France

Conducting and semi-conducting polymers are omnipresent in plastic electronics nowadays. Although structure-property correlations are central for device optimization, there is still insufficient understanding of the mechanisms and principles that govern thin film growth and chain packing, especially for the recent low band gap polymers of increasing molecular complexity e.g. p(NDIT2OD), PTB7, PCE11 and PCPDTBT. Crystallization/orientation of polymer semiconductors using epitaxy or high temperature rubbing is an elegant manner to tune their structure and organization that can further be investigated by transmission electron microscopy at different length scales. This contribution summarizes recent efforts of our group in this context and shows how the progress in mastering crystallization/orientation of semi-conducting polymers can be transposed to their conducting counterparts after soft doping. We demonstrate the possibility to fabricate highly oriented conducting polymer films whose charge conductivity and thermopower can reach beyond that of iodine-doped polyacetylene.

15 min. break

Invited Talk CPP 1.5 Mon 11:30 H14
Conjugated polymers: linking mesoscopic morphology and charge transport — ●DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We first discuss the complex relation between processing, polymorphism, and structure formation in several conjugated polymers: P3HT,¹ PCPDTBT,² and PBTTT.³ Their mesoscopic morphology, as elucidated by combining various experimental and atomistic simulation techniques, is used to explain particular features of charge carrier mobility.⁶ We then assess various strategies for in silico prediction of morphologies and electronic properties of conjugated polymers, starting solely from the chemical structure.^{4,5} Though it is too optimistic to say that we are approaching a true bottom-up multiscale modeling of conjugated polymers, the benefits from using computer simulations to complement experimental results are obvious.

¹ C. Poelking, D. Andrienko, *Macromolecules*, 46, 8941, 2013.

² F. Fischer, G. Schulz, D. Trefz, A. Melnyk, M. Brinkmann, D. Andrienko, S. Ludwigs, *Macromolecules*, 50, 1402, 2017.

³ A. Melnyk, M. Junk, M. McGehee, B. Chmelka, M. R. Hansen, D. Andrienko, *J. Phys. Chem. Lett.*, 8, 4155, 2017.

⁴ C. Scherer, D. Andrienko, *Eur. Phys. J. Spec. Top.*, 225, 1441, 2016.

⁵ P. Gemuenden, C. Poelking, K. Kremer, K. Daoulas, D. Andrienko, *Macromol. Rapid Commun.*, 36, 1047, 2015.

⁶ Sh. Ye, L. Janasz, W. Zajaczkowski, J. G. Manion, A. Mondal, T. Marszalek, D. Andrienko, K. Muellen, W. Pisula, D. S. Seferos, *Macromol. Rapid Commun.*, 1800596, 2018

CPP 1.6 Mon 12:00 H14
Engineering scale simulation of non-equilibrium network phases for battery electrolytes — ●LUDWIG SCHNEIDER and MARCUS MUELLER — Georg-August Universität Göttingen, Institute for Theoretical Physics, Göttingen, Germany

Diblock copolymer materials exhibit a rich equilibrium phase diagram, qualifying them for applications in fuel cells, filters, and battery materials. Self-assembly of these materials rarely results in the equilibrium structures. Instead, configurations are trapped in long-lived metastable states and can be stabilized via cross-linking or cooling below the glass transition temperature of one component. The properties of

these structures, such as ion-conductivity, can deviate from those of corresponding equilibrium phases.

SOMA, our massively-parallel implementation of the Single-Chain-in-Mean-Field (SCMF) algorithm, enables us to study systems with billions of particles and predict their structure formation, thus unraveling the transport properties of self-assembled diblock-copolymers as a function of volume fraction, f . Our investigations show that non-equilibrium morphologies exhibit a large scale fractal-like domain structure that influences the transport properties. The length scale of these structures highlight the necessity of large system sizes to obtain bulk properties. We quantify the transport via the tortuosity and the diffusion inside the network phase and show that equilibrium phases overestimate the transport capabilities of random networks.

CPP 1.7 Mon 12:15 H14

Multiscale modelling of multidimensional molecular architectures for efficient organic solar cells — MARVIN NYENHUIS, ●MARCUS BÖCKMANN, and NIKOS DOLTSINIS — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, Münster, Germany

The active layer of bulk hetero-junction (BHJ) organic solar cells

(OSCs) constitutes a complex mixture of polymeric donor (D) and acceptor (A) compounds [1] and its morphology is known to change upon *ad hoc* thermal annealing, thereby increasing the overall photo-conversion efficiency (PCE). While experimental techniques like STM or AFM yield but detailed information of the surface structure, we use multidimensional Molecular Dynamics simulations [2] to elucidate the interior constitution of the layer at the atomistic level. In this contribution, we present insight obtained recently for the interpretation of morphology related UV-vis spectra and domain formation [3,4] together with current results on a novel polymeric D/A mixture [5].

[1] A. J. Heeger, *Adv. Mater.* 2014, 26, 10. [2] M. Böckmann, D. Marx, C. Peter, L. Delle Site, K. Kremer, and N. Doltsinis, *Phys. Chem. Chem. Phys.* 2011, 10, 1039. [3] M. Böckmann, T. Schemme, D. de Jong, C. Denz, A. Heuer, and N. Doltsinis, *Phys. Chem. Chem. Phys.* 2015, 17, 28616. [4] T. Winands, M. Böckmann, T. Schemme, P. Ly, D. de Jong, Z. Wang, C. Denz, A. Heuer, and N. Doltsinis, *Phys. Chem. Chem. Phys.* 2016, 18, 6217. [5] D. Meng, H. Fu, C. Xiao, X. Meng, T. Winands, W. Ma, W. Wei, B. Fan, L. Huo, N. Doltsinis, Y. Li, Y. Sun, and Z. Wang, *J. Am. Chem. Soc.* 2016, 138, 10184.