

CPP 14: Poster Session II - Complex Fluids and Perovskites

Time: Tuesday 16:30–18:30

Location: CPPp

CPP 14.1 Tue 16:30 CPPp

Direct Observation of the Time-dependent Dynamic Tube Dilation in Entangled Polymer Blends — ●PAULA MALO DE MOLINA^{1,2}, ANGEL ALEGRÍA^{1,3}, JÜRGEN ALLGEIER⁴, MARGARITA KRUTEVA⁴, INGO HOFFMANN⁵, SYLVAIN PRÉVOST⁵, MICHAEL MONKENBUSCH⁴, DIETER RICHTER⁴, ARANTXA ARBE¹, and JUAN COLMENERO^{1,3,6} — ¹Materials Physics Center (CSIC-UPV/EHU), San Sebastian, Spain — ²IKERBASQUE - Basque Foundation for Science, Bilbao, Spain — ³Departamento de Física de Materiales (UPV/EHU), San Sebastian, Spain — ⁴Forschungszentrum Jülich GmbH, Jülich, Germany — ⁵Institut Laue-Langevin, Grenoble, France — ⁶Donostia International Physics Center, San Sebastián, Spain

The viscoelastic properties of high molecular weight polymers are given by their entanglement dynamics. In asymmetric polymer blends, the finite lifetime of constraints leads to a dilation of the tube but how does the tube dilate? The effective terminal tube dilation of the long chains can be determined from macroscopic techniques such as dielectric spectroscopy (DS) and rheology, which cannot resolve the time evolution of the tube diameter at the nm-scale. Here, we exploit (i) the possibility of isotopic (H/D) labeling and (ii) the spatial and time resolution of neutron spin echo (NSE) to directly probe the time-dependent tube dilation for long linear entangled chains in model blends with smaller isofrictional linear chains and small star polymers. By combining NSE with rheology and DS on the additive, the characteristic time that governs tube dilation is identified as the terminal time of the additive.

CPP 14.2 Tue 16:30 CPPp

Spray-deposited anisotropic ferromagnetic hybrid polymer films of PS-b-PMMA and strontium hexaferrite magnetic nanoplatelets — ●WEI CAO¹, SHANSHAN YIN¹, ANDREI CHUMAKOV², MATTHIAS OPEL³, MARKUS GALLEI⁴, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,5}, and PETER MÜLLER-BUSCHBAUM^{1,6} — ¹TU München, Physik-Department, 85748 Garching — ²DESY, 22607 Hamburg — ³WMI, Bayerische Akademie der Wissenschaften, 85748 Garching — ⁴Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — ⁵KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 44 Stockholm, Sweden — ⁶TU München, MLZ, 85748 Garching

Spray deposition is applied to fabricate anisotropic ferromagnetic hybrid polymer films by controlling the orientation of strontium hexaferrite nanoplatelets inside ultrahigh molecular weight diblock copolymer (DBC) polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) films. During spray deposition, the kinetics of structure evolution of the hybrid film is monitored in situ with grazing-incidence small-angle X-ray scattering. The obtained final hybrid film is then solvent annealed with tetrahydrofuran to study the influence of solvent vapor annealing (SVA). Due to the rearrangement of the nanoplatelets inside the DBC during SVA, an obvious change in the magnetic behavior of the hybrid film is observed. The hybrid film shows a perpendicular ferromagnetic anisotropy before SVA, which is strongly weakened after SVA. The spray deposited hybrid film appears highly promising for potential applications in magnetic data storage and sensors.

CPP 14.3 Tue 16:30 CPPp

Growth and morphology of sputtered iron layers on magnetic nanoparticle-containing diblock copolymer films — ●CHRISTOPHER EVERETT¹, MARTINA PLANK², MARKUS GALLEI³, MATTHIAS SCHWARTZKOPF⁴, STEPHAN ROTH^{4,5}, and PETER MÜLLER-BUSCHBAUM^{1,6} — ¹TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — ²TU Darmstadt, Ernst-Berl-Institute, Darmstadt, Germany — ³Saarland University, Chair in Polymer Chemistry, Saarbrücken, Germany — ⁴Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ⁵KTH Royal Institute of Technology, Stockholm, Sweden — ⁶Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

For highly functional magnetic sensors and high-density magnetic data storage, the exchange bias effect is of great technical importance. Exchange bias, typically observed at ferromagnetic/antiferromagnetic interfaces, has been reported in a variety of magnetic systems. In this investigation, ultra-high molecular weight polystyrene-block-poly(methyl methacrylate) (PS-b-PMMA) films with a large PS volume fraction are used as templates for ferrimagnetic magnetite (Fe₃O₄)

nanoparticles (NPs). Through solvent vapor annealing, nanostructured hybrid films with up to 5 wt % of NPs are obtained. The sputtering of iron (Fe), which is ferromagnetic, on the polymer template is monitored in situ with grazing incidence small-angle X-ray scattering (GISAXS). An analysis reveals that the growth of Fe on nanoparticle-containing diblock copolymer films is a complex process and is important in understanding the resulting magnetic properties.

CPP 14.4 Tue 16:30 CPPp

Micellization of a Multi-Responsive Triblock Terpolymers — ●YANAN LI¹, CHIA-HSIN KO¹, ATHANASIOS SKANDALIS², DMITRY MOLODENSKIY³, STERGIOS PISPAS², and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Physik weicher Materie, Garching, Germany — ²Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — ³EMBL at DESY, Hamburg, Germany

Triblock terpolymers having a hydrophobic, a thermo- and a pH- responsive block offer many possibilities for the formation of functional micelles and their manipulation by different environments. We investigate dual-stimuli-responsive micelles from poly(2-(dimethylamino) ethyl methacrylate)-b-poly(lauryl methacrylate)-b-poly(oligo(ethylene glycol) methyl ether methacrylate), PDMAEMA-b-PLMA-b-POEGMA [1]. The self-assembled micelles formed by these blocks can be applied in gene transfer and drug delivery applications. They consist of a strongly hydrophobic PLMA midblock, forming the core, and two biocompatible hydrophilic blocks, forming the shell. PDMAEMA is a weak cationic polyelectrolyte, which is both pH- and temperature-responsive. To avoid precipitation of the triblock terpolymers upon heating at high pH values, a third, permanently water-soluble, biocompatible POEGMA block is included to form triblock terpolymers. We investigate the temperature- and pH-dependent micellar structures as a function of polymer concentration by dynamic light scattering and synchrotron small-angle X-ray scattering. [1] A. Skandalis, S. Pispas, Polym. Chem. 2017, 8, 4538.

CPP 14.5 Tue 16:30 CPPp

Multi-dimensional morphology control for PS-b-P4VP templated mesoporous iron (III) oxide thin films — ●SHANSHAN YIN¹, WEI CAO¹, QING JI², YAJUN CHENG², LIN SONG³, NIAN LI¹, CHRISTIAN L. WEINDL¹, MATTHIAS SCHWARTZKOPF⁴, STEPHAN V. ROTH^{4,5}, and PETER MÜLLER-BUSCHBAUM^{1,6} — ¹Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — ²Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, P. R. China — ³Northwestern Polytechnical University, Xi'an 710072, China. — ⁴DESY, Notkestr. 85, 22603 Hamburg, Germany — ⁵Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — ⁶Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

We systematically investigate the synthesis of polystyrene-block-poly(4-vinylpyridine) templated Fe₂O₃ thin films by changing the solvent category (DMF or 1,4-dioxane) and the polymer-to-FeCl₃ ratios. DMF/1,4-dioxane mixtures with different component ratios are also prepared for revealing the effect of the solvent selectivity on the thin film morphology. The structure transition mechanism of the thin films is explained by the preferential affinity and the small-molecule surfactant micelles theory.

CPP 14.6 Tue 16:30 CPPp

In-situ spraying of Colloids on Cellulose Nanofibers — ●CONSTANTIN HARDER^{1,2}, MARIE BETKER^{1,3}, ALEXANDROS ALEXAKIS³, ANDREI CHUMAKOV¹, ELISABETH ERBES^{1,4}, MARC GENSCH^{1,2}, QING CHEN¹, JAN RUBECK¹, NILS LE COUTRE⁵, CALVIN J. BRETT^{1,3}, MATTHIAS SCHWARTZKOPF¹, EVA MALMSTRÖM³, DANIEL SÖDERBERG³, PETER MÜLLER-BUSCHBAUM², and STEPHAN V. ROTH^{1,3} — ¹Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany — ²Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ³KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden — ⁴Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Goettingen, Germany — ⁵Universität Rostock, Universität-

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Layer formation and annealing of colloidal inks applied to porous materials is very relevant for printing and functional coatings. The goal is to distinguish and quantify the differences in structure formation during annealing of deposited colloidal inks on a porous and a solid material. As porous template we use a layer of cellulose nano fibers (CNF) with a charged surface. We use novel colloidal inks consisting of poly-butylmethacrylate (PBMA) and poly-sobrerolmethacrylate (PSobMA) with a charged shell in aqueous solution. We studied the deposition and the subsequent structural and morphological changes during annealing of the colloidal layers in real-time using grazing incidence small-angle X-ray scattering (GISAXS). During deposition, we expect that part of the liquid enters the CNF layer while part of the solvent and the colloids remain on top of the nanopaper surface, leading to a complex drying process. Subsequently, the structural changes in the colloidal layer are induced by annealing. With GISAXS we monitor these different processes and their effect on the CNF template.

CPP 14.7 Tue 16:30 CPPp

Observing the role of β -lactoglobulin in biotemplating TiO₂ during spray deposition with in situ GIAX techniques: A route to green sol-gel chemistry — ●JULIAN E. HEGER¹, WEI CHEN¹, SHANSHAN YIN¹, CHRISTIAN L. WEINDL¹, CHRISTINA GEIGER¹, CALVIN J. BRETT^{2,3}, WIEBKE OHM³, STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — ²Royal Institute of Technology KTH, Teknikringen 34-35, 100 44 Stockholm, Sweden — ³Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — ⁴Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Polymer directed sol-gel chemistry provides a powerful way for a morphological tailored synthesis of titania, which can be subsequently spray deposited to form functional films. For a green chemistry approach, synthetic polymers are substituted with water-soluble biopolymers. In this work, we investigate the templating effect of β -lactoglobulin (β -lg), which is known to form different aggregates as a function of net charge controlled by pH during denaturation. For this, β -lg is mixed with an established titania precursor and denatured at a pH below its isoelectric point, to obtain hierarchical and crystalline titania at low-temperatures. Advanced in situ grazing incidence X-ray scattering (GIAX) synchrotron techniques identify the underlying kinetics of β -lg biotemplated titania films during spray deposition.

CPP 14.8 Tue 16:30 CPPp

Water dynamics in a concentrated aqueous solution of perdeuterated poly(N-isopropylacrylamide) across the cloud point — ●BAHAR YAZDANSHENAS¹, BART-JAN NIEBUUR¹, DIRK SCHANZENBACH², ANDRÉ LASCHEWSKY^{2,3}, MICHAELA ZAMPONI⁴, DARIA NOFERINI⁴, ALFONS SCHULTE⁵, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching — ²Universität Potsdam, Institut für Chemie — ³Fraunhofer IAP, Potsdam-Golm — ⁴FZ Jülich, JCNS at MLZ, Garching — ⁵University of Central Florida, Orlando, U.S.A.

In aqueous solutions of the thermoresponsive polymer poly(N-isopropylacrylamide) (PNIPAM), cooperative dehydration causes the polymer chains to collapse and aggregate at the demixing transition. Recent quasi-elastic neutron scattering (QENS) experiments have shown that the susceptibility spectra of hydration water occur at lower frequencies than those of bulk water and that their relative population decreases abruptly at the cloud point [1,2]. In the present study, we investigate the water dynamics on a perdeuterated PNIPAM sample in H₂O, down to ca. 0.08 GHz, using a combination of a high- and low-resolution QENS. Deuteration suppresses incoherent scattering from the polymer. In the observation window, we find two types of hydration water. 1. M. Philipp, C. M. Papadakis et al., J. Phys. Chem. B 2014, 118, 4253 2. B.-J. Niebuur, C. M. Papadakis et al., Macromolecules 2019, 52, 1942

CPP 14.9 Tue 16:30 CPPp

Co-nonsolvency induced collapse transition in thin PMMA-b-PNIPMAM films — ●JULIJA REITENBACH¹, CHRISTINA GEIGER¹, GAETANO MANGIAPIA², CRISTIANE HENSCHL³, ANDRÉ LASCHEWSKY³, CHRISTINE PAPADAKIS⁴, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching —

²Helmholtz-Zentrum Geesthacht am Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85748 Garching — ³Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm — ⁴TU München, Physik-Department, Physik weicher Materie, James-Franck-Str. 1, 85748 Garching

Thin films of the thermoresponsive diblock copolymer PMMA-b-PNIPMAM exhibit a co-nonsolvency induced collapse transition when organic cosolvents, like acetone or methanol, are introduced in a certain ratio into the surrounding vapor atmosphere. The macroscopic changes during the swelling in aqueous vapor and the collapse transition in cosolvent vapor mixtures are investigated with spectral reflectance (SR) and time-of-flight neutron reflectometry (ToF-NR) measurements. We reveal the solvent/cosolvent exchange taking place at the polymer functional groups with in situ Fourier-transform infrared spectroscopy (FTIR) and attribute key changes in the local chemical environment to the macroscopic film collapse stages.

CPP 14.10 Tue 16:30 CPPp

ToF-NR swelling study on metal coated PNIPAM microgel thin films using a 3D-printed environmental chamber — ●TOBIAS WIDMANN¹, LUCAS P. KREUZER¹, CHRISTINA GEIGER¹, JULIAN E. HEGER¹, GAETANO MANGIAPIA², THOMAS HELLWEG³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching — ²HZG at MLZ, 85748 Garching — ³Universität Bielefeld, Chemie Department, Physikalische und Biophysikalische Chemie, 33615 Bielefeld

Thermoresponsive microgels typically show a strong change in volume upon crossing the volume phase transition temperature (VPTT). For LCST type polymers, such as for example microgels based on N-isopropylacrylamide (NIPAM) which has an LCST of 32 °C, these microgels are in a hydrophilic state below the VPTT. In that temperature regime, they are highly sensitive to humidity, which makes them interesting candidates for humidity sensing applications on the nanoscale. Therefore, we investigate thin films of PNIPAM microgels cross linked with N,N*-methylenebisacrylamide under cyclic high and low humidity conditions. We follow the swelling and drying processes in situ using time-of-flight neutron reflectometry (ToF-NR). For that purpose, we used a custom made 3D-printed environmental chamber that was designed and built in the framework of the FlexiProb project, which aims for a quickly interchangeable sample environment for experiments at the European spallation source (ESS).

CPP 14.11 Tue 16:30 CPPp

Applications of Angular Cross-Correlation Analysis to Soft Matter — ●IVAN ZALUZHNYI¹, RUSLAN KURTA², MARCUS SCHEELE³, FRANK SCHREIBER¹, BORIS OSTROVSKII⁴, and IVAN VARTANYANTS^{5,6} — ¹Institute of Applied Physics, University of Tübingen, Tübingen, Germany — ²European XFEL, Schenefeld, Germany — ³Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — ⁴Federal Scientific Research Center "Crystallography and photonics", Moscow, Russia — ⁵Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ⁶National Research Nuclear University MEPhI, Moscow, Russia

An interesting feature of several soft matter systems is so-called orientational order, which can be referred to a specific orientation of anisotropic building blocks or bonds between these blocks. Angular x-ray cross-correlation analysis (AXCCA) is a method to analyze and interpret the anisotropy in x-ray scattering data in order to reveal the details of the orientational order [1]. In combination with scanning x-ray diffraction, AXCCA allows to study the spatial distribution of the orientational order across a large sample. After explaining the concepts of AXCCA, we will discuss the example of such a system, in which orientational order exists at several length scales, namely a superlattice of PbS nanocrystals coupled by organic linkers [2]. AXCCA allows to reveal the preferred orientation of nanoparticles with respect to the superlattice and the degree of angular disorder.

[1] I. Zaluzhnyy, et al., Materials 12 3464 (2019)

[2] I. Zaluzhnyy, et al., Nano Lett. 17 3511 (2017)

CPP 14.12 Tue 16:30 CPPp

Deformation and magnetic properties of clusters of supercolloidal magnetic polymers in microchannel under external field — ●VLADIMIR ZVEREV¹, EKATERINA NOVAK¹, SOFIA KANTOROVICH^{2,1}, and PEDRO SÁNCHEZ^{2,1} — ¹Ural Federal University, Ekaterinburg, Russia — ²University of Vienna, Vienna, Austria

Advances in synthesis technology in the field of magnetoreactive poly-

mer supracolloid structures (magnetic filaments) have reduced their characteristic sizes from a few micrometers to a nanoscale. Magnetic filaments are actively studied theoretically, in particular their magnetic response, rheological properties, which is important for predicting behavior in closed geometries, such as microchannels used in microfluidic devices. Microchannels are tubes whose size does not exceed hundreds of microns, and has several advantages, for example, a high speed of heat and mass transfer.

This work is devoted to the study of the effect of liquid flow and an external magnetic field on the cluster placed in the microchannel. Clusters are made from magnetic filaments that have chain, ring, X, and Y-like structures. It was found that the external magnetic field enhances the deformation of the cluster in the microchannel in a flow. Clusters can significantly change their shape, and they can also demonstrate oscillating in time magnetic response. The use of magnetic filaments in microchannels makes it possible to control hydrodynamic interactions in the microfluidic system using an external magnetic field. The work was supported by RSF 19-72-10033.

CPP 14.13 Tue 16:30 CPPp

Rheological properties of clusters of supracolloidal magnetic polymers in a microchannel — ●EKATERINA NOVAK¹, VLADIMIR ZVEREV¹, MARINA GUPALO¹, and SOFIA KANTOROVICH^{1,2} — ¹Ural Federal University, Ekaterinburg, Russia — ²University of Vienna, Vienna, Austria

Construction of supracolloidal magnetic polymers (polymer-like structures in which magnetic nanoparticles are playing the role of monomers) has recently been made possible. The advantage of such magnetic polymers is that they keep their structure independently from the temperature and that is why they can be potentially used as an alternative to nanoparticles in magnetic fluids to obtain a desired and easily controlled magnetic or rheological response. In this contribution, using Langevin dynamics simulations, we focused on solutions of filaments, the magnetic nanoparticles in which are not only interacting via dipole-dipole potential but also via short-range attractive forces (Lennard-Jones type). Such filaments tend to aggregate in dense spherical droplet-like clusters. The resulting composite soft colloid is placed in the microchannel, where its behavior in the shear flow is investigated, varying a wide range of system parameters. We find that with time the cluster gets elongated. The higher is the shear rate the faster the flow can deform the cluster. The work was supported by RSF 19-72-10033.

CPP 14.14 Tue 16:30 CPPp

Influence of monomers on the self-assembly of supramolecular magnetic polymers — ●ELENA PYANZINA, ANNA AKISHEVA, EGOR NAUMOV, and EKATERINA NOVAK — Ural Federal University, Ekaterinburg, Russia

In this paper, an analysis of the qualitative change in equilibrium properties with temperature, at different lengths of the polymer and the parameters of the dipole-dipole interaction was carried out. As comparative characteristics were used: the radius of gyration, magnetic moment, form factor and anisotropy of the shape of the polymer. Both individual configurations were considered, and the best types of each filament were identified, and a general comparison of the filaments was made. The main objective of our work is to study the qualitative structural change in the behaviour of the filament when particle's size and shape are introduced in various polymer configurations.

This work was supported by RSF grant * 19-72-10033.

CPP 14.15 Tue 16:30 CPPp

Investigation of polymer templated Silicon-Germanium hybrid materials — ●CHRISTIAN L. WEINDL¹, CHRISTIAN FAJMAN², MICHAEL A. GIEBEL², MATTHIAS SCHWARZKOPF³, STEPHAN V. ROTH^{3,4}, THOMAS F. FÄSSLER², and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹Technische Universität München, PhysikDepartment, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — ²Technische Universität München, Chemie-Department, Lehrstuhl für anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching, Germany — ³Deutsches Elektronen-Synchrotron DESY, Noetkestraße 85, 22607 Hamburg, Germany — ⁴Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — ⁵Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The latest research has revealed promising results for Silicon (Si) and Germanium (Ge) as anode materials for lithium-ion batteries. Owing

to their high energy capacity these two semiconductors are considered auspicious alternatives to graphite anodes. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a wet chemical sol-gel approach. Here, diblock copolymer polystyrene-block-polyethylene oxide is used as the structuring agent. Real-space data as SEM and microscopy images will be discussed with reciprocal-space analysis methods as grazing-incidence x-ray scattering in small and wide-angle mode.

CPP 14.16 Tue 16:30 CPPp

A Further Step Towards Space: Perovskite and Organic Solar Cells on a Rocket Flight — ●LENNART REB¹, MICHAEL BÖHMER², BENJAMIN PREDESCHLY¹, SEBASTIAN GROTT¹, CHRISTIAN WEINDL¹, GORAN IVANDEKIC¹, RENJUN GUO¹, CHRISTOPH DREISSIGACKER³, ROMAN GERNHÄUSER², ANDREAS MEYER³, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — ²TU München, Physik-Department, Zentrales Technologielabor, Garching, Germany — ³Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, Germany — ⁴Heinz Maier-Leibniz-Zentrum, Garching, Germany

Perovskite and organic solar cells possess a revolutionary potential for space applications. The thin-film technologies enable an exceptional power per mass, exceeding herein their inorganic counterparts by magnitudes. However, research was mainly restricted to terrestrial conditions so far. We report the launch of two types of perovskite and organic solar cells on a suborbital rocket flight, possibly the first in-situ demonstration of these technologies in space conditions [1]. Both, planar and mesoscopic nip-type perovskite solar cell types exceeded an power per area of 14 mW cm⁻², whereas both bulk heterojunction absorber PBDB-T:ITIC and PTB7-Th:PC71BM organic solar cell types reached more than 4 and 7 mW cm⁻², respectively. Our results highlight both the suitability for near-Earth applications and the potential for deep space missions of these technologies. [1] L. Reb et al., *Joule* 4,1880-1892 (2020), doi.org/10.1016/j.joule.2020.07.004.

CPP 14.17 Tue 16:30 CPPp

Tuning ordered mesoporous titania films via introducing germanium nanocrystals for high-efficient photoanodes — ●NIAN LI¹, RENJUN GUO¹, WEI CHEN¹, VOLKER KÖRSTGENS¹, JULIAN E. HEGER¹, SUZHE LIANG¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg

With an aim of obtaining high-efficient titania photoanodes, we introduce germanium nanocrystals (GeNCs) into a diblock-copolymer template-assisted sol-gel synthesis. The surface and inner morphologies of the TiO₂/GeNC films with different GeNC content after thermal annealing are investigated via scanning electron microscopy and grazing incidence small-angle X-ray scattering (GISAXS). We also probe the crystal phase, chemical composition and optical properties of the nanocomposite films via X-ray diffraction, transmission electron microscopy, X-ray photoelectron spectroscopy and ultraviolet-visible spectroscopy. These measurements show that even with GeNC addition, the nanocomposite films still have ordered nanostructures, good crystallinity and high transparency. We further study the charge-carrier dynamics of the nanocomposite films. Compared to pristine titania photoanodes, the GeNC addition enhances the electron transfer, resulting in an overall improvement in the short-circuit current density (J_{sc}) of the exemplary perovskite solar cells and thereby an enhanced solar cell efficiency.

CPP 14.18 Tue 16:30 CPPp

Degradation mechanisms of perovskite solar cells under different atmospheres — ●RENJUN GUO¹, DAN HAN², WEI CHEN¹, LINJIE DAI³, KANGYU JI³, QIU XIONG⁴, SAISAI LI⁵, LENNART K. REB¹, MANUEL A. SCHEEL¹, SHAMBHAVI PRATAP¹, NIAN LI¹, SHANSHAN YIN¹, TIANXIAO XIAO¹, SUZHE LIANG¹, ANNA-LENA OECHSLE¹, CHRISTIAN L. WEINDL¹, MATTHIAS SCHWARZKOPF⁶, HUBERT EBERT², PENG GAO⁴, MINGJIAN YUAN⁵, NEIL C. GREENHAM³, SAMUEL D. STRANKS³, STEPHAN V. ROTH⁶, RICHARD H. FRIEND³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München — ²James-Franck-Str. 1 — ³University of Cambridge — ⁴Chinese Academy of Sciences — ⁵Nankai University — ⁶Deutsche Elektronen-Synchrotron

We investigate degradation mechanisms of perovskite solar cells under different atmospheres via in-situ grazing-incidence X-ray scattering methods. We reveal that the atmosphere has a significant influence on

degradation mechanisms for materials. This results in the degradation of the performances of the relative perovskite solar cells. Compared with the performance evolution of perovskite solar cells under vacuum, they show better stability under nitrogen.

CPP 14.19 Tue 16:30 CPPp

Fabrication of Plasmonic Nanostructures for Perovskite Solar Cells — •TIANFU GUAN, RENJUN GUO, SUZHE LIANG, NIAN LI, CHRISTIAN L. WEINDL, WEI CAO, and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany

Plasmonic metal-dielectric composites have fascinated a great interest in various fields, owing to surface plasmon resonance (SPR) induced by incident radiation. The utilization of plasmonic metal nanoparticles (NPs) is frequently proposed as a means to further enhance the light absorption in the broad wavelength range as well as to facilitate charge collection and transport in the Perovskite solar cells (PSCs). To regulate the plasmonic spectral of Au NPs for maximizing the enhancement in light-absorption of the photoactive layer, we assembly the metal NPs onto the electron collecting layer to broaden the absorption band of the photoactive layer of optoelectronic devices as well as enhance the device performance. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density, and morphology of the Au NPs will influence the crystallinity of the perovskite film and charge transportation of the device. Besides, grazing incidence small angle x-ray scattering (GISAXS) is used to study the quality of the plasmonic structure interface in terms of contact area between the perovskite film. Grazing incidence wide angle x-ray scattering (GIWAXS) is used to probe the crystalline structure of the perovskite active layers.

CPP 14.20 Tue 16:30 CPPp

Mesoporous ZnO thin films templated by diblock copolymer for photovoltaic applications — •TING TIAN and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Mesoporous ZnO thin films have received tremendous attention in photovoltaic applications in view of their high electron mobility, high transparency, high surface area, and the superior ability to host the light-harvesting dyes and the organic molecular hole-transporters. Considering the morphology-dependent device performance, a precise control over the ZnO nanostructures is indispensable. Among the existing synthesis routes, the diblock copolymer assisted sol-gel approach has been corroborated to be powerful and promising in morphology tunability. Benefiting from the solution processability, this wet chemical method can be integrated into industry-based processes and thus achieve large-scale, high-throughput production. In the present work, an amphiphilic diblock copolymer is used as the structure-directing agent and slot-die coating is applied as the deposition technique to fabricate the mesoporous ZnO films. Effects of ZnO precursor variables on morphological evolution of mesoporous ZnO films are systematically investigated. The generated nanostructures on the film surface are detected by surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by reciprocal-space Grazing-incidence small angle X-ray scattering (GISAXS) technique.

CPP 14.21 Tue 16:30 CPPp

The Role of CsBr in Crystal Orientation and Optoelectronic Properties of MAPbI₃-based devices — YUQIN ZOU and •PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany.

Orientations of crystal planes impact on the behavior of photogenerated charge carriers and are vital for developing electronic properties of the corresponding devices. Herein, we propose a facile approach to reveal the effect of crystal stacking on the charge carrier kinetics by doping CsBr to enable the formation of a mix-cations perovskite phase. We use grazing-incidence wide-angle X-ray scattering to probe the crystal structure and crystal orientation of the mixed perovskite thin films revealing the effect of the extrinsic CsBr doping on the stacking of the crystal planes. TPV, TPC and tDOS are also used to detect the recombination of the photo-generated charge carriers and the trap-state density. It is demonstrated that CsBr compositional engineering can effectively tune the crystallization orientation of crystal planes, reduce trap-state density and facilitate photocarriers transport across

the absorber and pertaining interface simultaneously. This strategy provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport and the optoelectronic properties of solar cells.

CPP 14.22 Tue 16:30 CPPp

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CPP 14.23 Tue 16:30 CPPp

Energetics of lead halide perovskite precursors in different solvents — •RICHARD SCHIER¹, ANA M. VALENCIA², and CATERINA COCCHI² — ¹Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin — ²Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg

Lead halide perovskites (LHPs) are an emerging class of solution-processed materials with excellent photovoltaic performance. The characterization of LHP precursors in solution is a lively field of research [1,2]. The goal of this work is to understand the formation and stability of LHP precursors with chemical formula PbX₂M₄, where X = Cl, Br, I, and M = ACN, DMF, DMSO, GBL, NMP, PC are common solvents. In the framework of density functional theory coupled to the polarizable continuum model to implicitly simulate the solvent cavity, we calculate and analyze the energetics, the structural properties, and the charge distribution in all these systems. Our calculated formation energies are qualitatively in agreement with earlier reports in the literature [1]. With this systematic study we are able to capture general trends: heavier halide species lead to a lower formation energy; the explicit solvent exerts a clear influence on the energetics, on the Pb-X bond lengths and angle, and on the charge distribution within the complexes.

[1] Radicchi et al., ACS Appl. Energy Mater. 2, 3400 (2019)

[2] A.M. Valencia et al., arXiv2012.08440

CPP 14.24 Tue 16:30 CPPp

Imaging ferroelastic domains in MAPbI₃ perovskite via dual frequency resonance tracking PFM — •ILKA HERMES¹ and RO-MAIN STOMP² — ¹Park Systems Europe, Mannheim, Germany — ²Zuerich Instruments, Zuerich, Switzerland

Methylammonium lead iodide (MAPbI₃)-based photovoltaics have seen an astonishing increase in efficiency due to their unique optoelectronic properties and charge carrier dynamics. Since MAPbI₃ crystallizes in a tetragonal perovskite structure, researchers have long suggested that the material features ferroelectricity and -elasticity. These ferroic properties are thought to influence the charge carrier dynamics in MAPbI₃ photovoltaics and, therefore, require accurate characterization on the nanoscale, available via piezoresponse force microscopy (PFM). On thin films, a weak piezoresponse often has to be enhanced by driving the electrical excitation of PFM close to the contact resonance of the cantilever. However, the contact resonance depends on a consistent tip-sample contact. Therefore, a high surface roughness or nanomechanical heterogeneities can introduce crosstalk, which exacerbates the data interpretation of the electromechanical sample response. Dual frequency resonance tracking (DFRT) improves the stability of the resonance enhancement via an additional frequency feedback that compensates for shifts in the contact resonance. Here, we demonstrate that DFRT-PFM, available by combining Park Systems atomic

force microscopes with Zurich Instruments lock-in amplifiers, not only reduces crosstalk, but also resolves the mechanical contrast on ferroelastic MAPbI₃ domains.

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In situ phase and texture evolution tracking of the formation of 2-step slot-die coated perovskite by GIWAXS — •MANUEL A. SCHEEL¹, LENNART K. REB¹, RENJUN GUO¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹Lehrstuhl für Funktionelle Materialien, Physik-Department — ²DESY, Notkestr. 85, 22607 Hamburg — ³KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — ⁴Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite slot-die coating is a particularly promising deposition technique for hybrid perovskite materials. With the perovskite absorber being the key material in a perovskite-based solar cell, structure and morphology control during thin-film formation is essential in achieving highly homogeneous and thus high-performing layers. To better understand morphology evolution and crystallization kinetics during film formation, we investigate the conversion of slot-die coated lead iodide and slot-die coated methylammonium iodide to perovskite by in situ grazing-incidence wide-angle X-ray scattering (GIWAXS). In this work we study the thin-film morphology and texture evolution during the conversion process triggered by thermal annealing. We track the phase

evolution and their respective crystal orientations over time. As a reference, we investigate spin-cast PbI₂, MAI and MAPbI₃ thin-films and look into methodical differences that can influence the film quality.

CPP 14.26 Tue 16:30 CPPp

Optical properties and structure-property relations of lead halide perovskite building blocks in solution — •GIOVANNI PROCIDA¹, RICHARD SCHIER², ANA VALENCIA^{1,2}, and CATERINA COCCHI^{1,2} — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg — ²Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin

Hybrid metal-halide perovskites are among the best solution-processed currently available. Characterizing the optical properties of their building blocks in different solvents is of great relevance to link the behavior of the precursors to the final thin films. Here, we focus on PbX₂(Sol)₄ compounds in solution, where X=Cl, Br, and I, and Sol=DMSO, GBL, ACN, DMF, PC, NMP, and, in the first-principles framework of time dependent density functional theory coupled to the polarizable continuum model, we unravel their electronic and optical properties. We find that the energy of the frontier orbitals is modulated by the choice of the solvent. Specifically, electron-withdrawing groups lead to a downshift of both HOMO and LUMO while electron-donating groups give rise to the opposite effect. We also find dependence of the band-gap on the halide species, which in turns influences the energy of the absorption onset.