

CPP 8: Poster Session III

Active Matter (1-2); 2D Materials (3); Biopolymers, Biomaterials and Bioinspired Functional Materials (4-7); Charged Soft Matter, Polyelectrolytes and Ionic Liquids (8-12); Composites and Functional Polymer Hybrids (13); Hydrogels and Microgels (14); Interfaces and Thin Films (15-27); Nanostructures, Nanostructuring and Nanosized Soft Matter (28); Responsive and Adaptive Systems (29-32).

Time: Wednesday 17:30–19:30

Location: P

CPP 8.1 Wed 17:30 P

Janus Particles Self-Assembly: Magnetic and Catalytic Propulsion of Clustered Janus Particles — ●YARA ALSAADAWI¹, ANNA EICHLER-VOLF¹, MICHAEL HEIGL², PETER ZAHN¹, MANFRED ALBRECHT², and ARTUR ERBE¹ — ¹Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — ²Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Janus particles are one type of artificial microswimmers consisting of two asymmetrically functionalized surfaces. With proper manipulation, one can control their movement from one point to another at certain velocities, as well as clustering, and orientations. In this work, we prepared Janus particles with caps consisting of Co/Pd, providing magnetic and H₂O₂ catalytic activity for particle propulsion. Due to their magnetic properties, individual particles undergo self-assembly by cap-cap interactions, forming clusters with varying sizes and shapes. Here, we observed clusters of two- and three-janus particles with standard video microscopy. Furthermore, the influence of external magnetic field on a cluster propulsion was studied, as well as the effect of propulsion next to a wall. We reported varying propulsion trajectories, which in turn depend on the number of particles and the cap-cap arrangement within a cluster.

CPP 8.2 Wed 17:30 P

Analytical study of active semiflexible ring polymer — ●CHRISTIAN ANTON PHILIPPS, ROLAND GEORG WINKLER, and GERHARD GOMPPER — Forschungszentrum Jülich Institute of Biological Information Processing, Jülich, Germany

Nature provides a variety of active matter systems, with self-propelled agents consuming internal energy or extracting it from their vicinity for locomotion [1]. Examples on the cellular level are self-propelled semiflexible actomyosin ring-like filaments driven by myosin motors in the cytoskeleton. We present a theoretical study of an active ring polymer [2] with tangential propulsion, applying the continuous Gaussian semiflexible polymer model [3] and introducing periodic boundary conditions. By a normal-mode expansion, the ring polymer conformational and dynamical properties, emerging by the homogeneous active force and its interplay with rigidity, are determined. Remarkably, the ring conformations are unaffected by activity for any stiffness. In contrast to linear filaments, the center-of-mass motion is independent of propulsion. However, activity strongly influences the internal dynamics with a dominant rotational mode over several orders of magnitude in time for high activities. This corresponds to a rotational motion of the entire ring polymer. [1] R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. 86, 101014 (2017); [2] M. Mousavi, R. G. Winkler, G. Gompper, J. Chem. Phys. 150, 064913 (2019); [3] T. Eisenstecken, G. Gompper, R. G. Winkler, Polymers 8, 304 (2016).

CPP 8.3 Wed 17:30 P

Predicting the bulk modulus of single-layer 2D COFs from their molecular building-blocks properties — ●ANTONIOS RAPTAKIS^{1,2}, ALEXANDER CROY¹, AREZOO DIANAT¹, RAFAEL GUTIERREZ¹, and GIANAURELIO CUNIBERTI¹ — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — ²Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str.

Two-dimensional Covalent Organic Frameworks (2D COFs) have attracted a lot of interest due to their large range of potential applications. Bottom-up engineering of their molecular building-blocks can lead to novel structures with fine-tuned physical and chemical properties. We have carried out a computational investigation of the elastic properties of different 2D COFs with square and hexagonal lattices. Specifically, the 2D bulk modulus and equivalent spring constants of the respective molecular building-blocks were calculated. Considering the material as a spring network, an analytical model for each topology was derived, which can be used to predict the 2D bulk modulus based

on the properties of the monomeric units.

CPP 8.4 Wed 17:30 P

The possibility of spray coating of lignin and characterization of the thin film — ●SOPHIE SNOKE^{1,2,3}, CONSTANTIN HARDER^{1,4}, WIENKE REYNOLDS², and STEPHAN V. ROTH^{1,5} — ¹Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — ²Lignopure GmbH, 21073 Hamburg — ³Institute of Thermal Separation Processes, Technische Universität Hamburg-Harburg, 21073, Hamburg, Germany — ⁴Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — ⁵KTH Royal Institute of Technology, 100 44 Stockholm, Sweden

Lignin is a binding agent in wood and very promising regarding the sustainable development of new bio-based applications. Therefore, three different lignins were tested for spray coating. The lignin was dissolved in two different solvent mainly in Aceton and Tetrahydrofuran. The structure and morphology as well as the crystallinity of the lignin thin films were investigated by using grazing incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS). Through atomic force microscopy (AFM) the surface morphology and film thickness were characterized. The first goal is to discover possible applications of lignin in thin film applications by the usage of spray coating. The second one is to characterize the molecular and nonoscale arrangement of lignin in thin films.

CPP 8.5 Wed 17:30 P

Inorganic-organic hybrid nanostructures based on biopolymer templating — ●LINUS FIDELIS HUBER and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Inorganic-organic hybrid nanostructures are researched for many different applications. This work is focused on energy conversion through the thermoelectric effect, where electrical current can be generated from a temperature difference. However, the state of the art thermoelectric generators (TEG) often use materials like bismuth (Bi), tellurium (Te), antimony (Sb) or lead (Pb). These materials are toxic and expensive, giving rise to a need for a cleaner and more abundant alternative that still produces good conversion efficiencies. The efficiency of materials to produce thermoelectric power is mainly governed by three factors. The Seebeck coefficient, the electrical conductivity and the thermal conductivity. These parameters can be improved by changing the material morphology. For example, a sufficient percolation network can increase electrical conductivity. Beta-lactoglobulin is a bovine whey bio-polymer, that is known to form different aggregates under different environmental conditions. This material is used to structure and improve the performance of titania films. The differently structured beta-lactoglobulin-titania thin-films are studied with AFM and SEM as well as the Seebeck coefficient, thermal conductivity and electrical conductivity are measured using a 4-point probe setup.

CPP 8.6 Wed 17:30 P

Protein-polysaccharide nanoparticles stabilized by thermal treatment — ●JOHANNES ALLWANG¹, YANAN LI¹, STEFANO DA VELA², DIMITRIS SELIANITIS³, ANGELIKI CHRONI³, ARISTEIDIS PAPAGIANNOPOULOS³, and CHRISTINE M. PAPADAKIS¹ — ¹Physics Department, Technica University Munich, Garching, Germany — ²EMBL, DESY, Hamburg, Germany — ³Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

Protein complexes appear in healthy and diseased life forms as well as in food systems and medical applications. Their study can, therefore, give vital insights into biological mechanisms and help understand and treat diseases. Thermal treatment of protein-polysaccharide complexes was shown to create tunable nanoparticles with potential applications as carriers for nutrients and drugs [1].

Here, we investigate nanoparticles from trypsin; a proteolytic en-

zyme from the small intestine [2]. We use two different polysaccharides: hyaluronic acid and chondroitin sulfate. Synchrotron small-angle x-ray scattering is combined with light scattering methods to get insight into both the internal structure of the particles and their overall size.

[1] A. Papagiannopoulos, E. Vlasi, A. Radulescu, *Carbohydr. Polym.* **2019**, 218, 218

[2] S. Trampari, A. Papagiannopoulos, S. Pispas, *Biochem. Biophys. Res. Commun.* **2019**, 515, 282

CPP 8.7 Wed 17:30 P

Colloidal layer formation and imbibition of colloidal inks on and in thin cellulose films — ●CONSTANTIN HARDER^{1,2}, MARIE BETKER^{1,3}, ALEXAKIS E. ALEXAKIS³, ANDREI CHUMAKOV¹, BENEDIKT SOCHOR¹, ELISABETH ERBES^{1,4}, MARC GENSCH^{1,2}, QING CHEN¹, JULIAN HEGER², JAN RUBECK¹, CALVIN BRETT^{1,3}, MATTHIAS SCHWARTZKOPF¹, EVA MALMSTRÖM³, DANIEL SÖDERBERG³, PETER MÜLLER-BUSCHBAUM², and STEPHAN ROTH^{1,3} — ¹DESY, Hamburg, Germany — ²Lehrstuhl für Funktionelle Materialien, TUM, Garching, Germany — ³KTH, Stockholm, Sweden — ⁴Institute for X-ray Physics, Goettingen University, Goettingen, Germany

Layer formation and annealing of nanoparticles especially colloidal inks applied to porous materials is very relevant for functional coatings and printing. The goal is to distinguish and quantify the differences in structure formation during annealing of deposited colloidal inks on a porous material. Therefore, we use layers of cellulose nano fibers (CNF) as porous media. We use novel colloidal inks consisting of polybutylmethacrylate (PBMA) and poly-sobrolmethacrylate (PSobMA) in aqueous solution. We studied the deposition and the subsequent structural and morphological changes during annealing of the colloidal layers in real-time. During deposition 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. Our results show that the CNF- and colloidal layer will change if the glass transition temperature of the colloids is exceeded.

CPP 8.8 Wed 17:30 P

Conformation and packing of polyanions in polyelectrolyte complexes - a combined PFG and solid-state NMR study — BENJAMIN KOHN, CAROLIN NAAS, UWE LAPPAN, and ●ULRICH SCHELER — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Polyelectrolyte complexes find wide applications in surface modification and controlled drug delivery. In the highly charged states direct ion pairing between polycation and polyanion is expected. The conformation of a weak polyanion depends on pH and ionic strength. The effective charge is determined from electrophoresis NMR, PFG NMR yields the hydrodynamic size as a measure for the conformation. Separating 1H MAS spectra in two-dimensional single-quantum-double-quantum correlation spectra identifies acid protons hydrogen bonded to other acid protons and thus and polyanion-rich regions in the complexes. At low pH this is reduced by a factor of three in the complexes compared to the pure polyanion. At higher pH (high nominal charge) with a more stretched conformation almost none acid-acid contacts are found in the complexes. In the 22Na spectra signals from NaCl and sodium maleate are distinguished and quantified. Even at the highest pH when all of the polyanion is dissociated about one quarter of the sodium is detected in maleate in the complexes. This extrinsic charge compensation shows that in any case there is no straight ion pairing between the polycation and polyanion, phases of pure polyanion remain.

CPP 8.9 Wed 17:30 P

Dielectric spectroscopy on lithium-salt-based deep eutectic solvents — ●ARTHUR SCHULZ, PETER LUNKENHEIMER, and ALOIS LOIDL — University Augsburg, Experimental Physics V

Lithium-salt-based deep eutectic solvents, where the only cation is Li⁺, are promising candidates as electrolytes in electrochemical energy-storage devices like batteries. We have performed broadband dielectric spectroscopy on three such systems, covering a broad temperature and frequency range that extends from the low-viscosity liquid around room temperature down to the glassy state approaching the glass-transition temperature. We observe a relaxational process that can be ascribed to dipolar reorientational dynamics and exhibits the clear signatures of glassy freezing. We find that the temperature dependence of the ionic dc conductivity and its room-temperature value also are governed by the glassy dynamics of these systems, depending, e.g., on the

glass-transition temperature and fragility. Compared to previously investigated systems, containing the same hydrogen-bond donors and choline chloride instead of a lithium salt, both the reorientational and ionic dynamics are significantly reduced due to variations of the glass-transition temperature and the higher ionic potential of the lithium ions. These lithium-based deep eutectic solvents partly exhibit significant decoupling of the dipolar reorientational and the ionic translational dynamics and approximately follow a fractional Debye-Stokes-Einstein relation, leading to an enhancement of the dc conductivity, especially at low temperatures.

CPP 8.10 Wed 17:30 P

Poly((trifluoromethane)sulfonimide lithium styrene) as solid polymer electrolyte for lithium-ion batteries — ●FABIAN ALEXANDER CHRISTIAN APFELBECK¹ and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technische Universität München, Physik Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — ²Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Garching, Germany

Lithium-ion batteries turned out as an indispensable energy supplier in modern society which however suffers from safety concerns due to the flammability of the liquid electrolyte. Solid polymer electrolytes (SPEs) can bypass this obstacle and therefore represent a serious alternative to conventional electrolytes. Especially single-ion conducting polymers (SICPs), which have the anion covalently bonded to the backbone of the polymer and thus exhibit a theoretical transference number of unity, are of great interest in battery research. This property is especially interesting for lithium metal batteries due to the ability of suppressing dendritic growth. In addition to that, these polymers show reasonable high ionic conductivities (10^{-4} S cm⁻¹ at room temperature) compared to common electrolytes, what makes commercialization possible. Here, the SICP Poly((trifluoromethane)sulfonimide lithium styrene) (PSTFSLi) with Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) is used as SPE and capillary battery cells are fabricated and tested. This special cell type allows the observation of the structural evolution of the polymer electrolyte during cycling of the battery with small/wide angle x-ray scattering (SAXS/WAXS).

CPP 8.11 Wed 17:30 P

Influence of Mg on the structure and electrolyte/electrode interface in all-solid-state lithium battery — ●YUXIN LIANG and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Frank-Str.1, 85748 Garching, Germany

The interest in all-solid-state lithium battery mainly stems from its high safety and energy density compared with conventional Li-ion batteries. Solid polymer electrolytes (SPEs) as an essential component with high durability, long shelf life, high energy density, great flexibility for cell design and light in weight are considered as the most promising material for the next generation batteries. However, as the most common SPE, poly(ethylene oxide) (PEO) electrolytes have limited electrochemical windows and can react with lithium metal to form a solid electrolyte interphase (SEI), meaning that such SPE is more instable in high-energy-density batteries. Moreover, inhomogeneity at the electrolyte/electrode interface, with or without a SEI, can elicit an irregular lithium plating that leads to dendrite formation, resulting in the cycle life reduction and total cell resistance increase. As a modifying strategy, adding inorganic particles can alter the degree of non-conducting crystalline polymer volume within the electrolyte, promote the dissociation of Li⁺-TFSI⁻ ion pairs and increase the amount of mobility Li⁺ ions. Herein, Mg(ClO₄)₂ is introduced to the PEO electrolyte to modify the structure of SPE and increase the ionic conductivity. Besides, the additive can also assist in constructing a Li⁺-conducting SEI at the electrolyte/electrode interface.

CPP 8.12 Wed 17:30 P

Poly(propylene carbonate) as a solid polymer electrolyte — ●THIEN AN PHAM^{1,2}, RALPH GILLES¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Garching, Germany — ²Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany

Li dendrite growth was identified as one of the main obstacles preventing Li metal as anode material in commercial batteries with liquid electrolytes since it can cause short circuits, and, ultimately, generate safety concerns. By using solid polymer electrolytes (SPE), the safety of the lithium-ion battery cell can be increased since they offer higher

mechanical stability impeding Li dendrite growth. There has been a lot research on poly(ethylene oxide) (PEO) based SPE for the use with Li metal anodes since it offers high ionic conductivity. However, PEO is only stable up to potentials of 4V and thus, cannot be used with state of the art cathode materials like $\text{LiNi}_{1-x-y}\text{Mn}_x\text{Co}_y\text{O}_2$ that normally are operated at voltages above 4V. Aliphatic polycarbonates such as poly(ethylene carbonate) (PEC) or poly(propylene carbonate) (PPC) have intrinsically higher oxidation voltages than PEO making them suitable for high energy cathodes. Here, thin PPC films with different amount of Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt are prepared via drop casting method and studied with electrochemical impedance spectroscopy in order to determine the ionic conductivity.

CPP 8.13 Wed 17:30 P

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 SCHARTZKOPF⁴, 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 $\alpha\text{-Fe}_2\text{O}_3$ thin films by changing the solvent category (DMF or 1,4-dioxane) and the polymer-to- FeCl_3 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 8.14 Wed 17:30 P

Magnetic response of CoFe_2O_4 nanoparticles confined in PNIPAM-microgel networks — ●JOACHIM LANDERS¹, MARCUS WITT², JURI KOPP¹, STEPHAN HINRICH³, SOMA SALAMON¹, BIRGIT HANKIEWICZ³, REGINE VON KLITZING², and HEIKO WENDE¹ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen — ²Department of Physics, TU Darmstadt — ³Institute of Physical Chemistry, Hamburg University

Magnetic microgels of CoFe_2O_4 nanoparticles embedded in N-isopropylacrylamid (NIPAM) hydrogel exhibit versatile response behavior to external stimuli, combining the characteristic NIPAM volume phase transition (VPT) with tunable response to external magnetic fields determined by the local surrounding of the magnetic nanoparticles. In addition to conventional magnetic microgels, samples modified with allyl mercaptan affecting their swelling behavior were examined regarding their internal structure and magnetization dynamics. For an in-depth analysis of the nanoparticle confinement governing the microgels' magnetic response, detailed mappings of frequency- and temperature-dependence of the microgels' magnetic AC-susceptibility were recorded, enabling the precise resolution of Néel-type and Brownian dynamics as well as the extraction of nanoparticle confinement parameters. We observe a distinct reaction of nanoparticle dynamics across the VPT, showing characteristic differences when comparing conventional and allyl mercaptan - modified microgels. Funding by the DFG via SPP 1681 (project WE 2623/7-3, FI 1235/2-2 and KL 1165/18-1) is gratefully acknowledged.

CPP 8.15 Wed 17:30 P

2D covalent organic frameworks on monolayer MoS₂ — ●WENBO LU¹, DAVOR ČAČPETA², MIHAELA ENACHE¹, and MEIKE STÖHR¹ — ¹Zernike Institute for Advanced Materials, University of Groningen, Netherlands — ²Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have received increasing attention as promising materials for different applications. One possibility to precisely tune the electronic and optical properties to the desired applications is based on adsorbing well-ordered organic assemblies on TMDs. Here, a study of on-surface

synthesis of 2D covalent organic frameworks (COFs) on monolayer molybdenum disulfide (MoS_2) on highly oriented pyrolytic graphite (HOPG) will be presented. Monolayer MoS_2 films were synthesized by chemical vapor deposition and transferred to HOPG. The transferred MoS_2 was characterized by atomic force microscopy and scanning tunneling microscopy (STM), from which we conclude that the transferred MoS_2 is of high-quality with micrometer sized domains. For 2D COF formation, 1,4-benzenediboronic acid (BDBA) was deposited onto the MoS_2 /HOPG. The structure of the formed 2D COFs was studied via STM. The dehydration of BDBA results in the formation of a long-range ordered honeycomb molecular network on MoS_2 . Our results show the possibility of using 2D COFs to build up ordered organic/2D TMDs interfaces, which is promising for the fabrication of hybrid organic-inorganic devices possessing tailored properties.

CPP 8.16 Wed 17:30 P

PbS quantum dot solar cells via hybrid interfacial architecture — HUAYING ZHONG¹, WEI CHEN^{1,2}, and ●PETER MÜLLER-BUSCHBAUM^{1,3} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²Southern University of Science and Technology (SUSTech), Department of Electrical and Electronic Engineering, 1088 Xueyuan Avenue, 518055 Shenzhen, P.R. China — ³Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Colloidal quantum dots (CQDs) have generated great interest in various optoelectronic devices because of their size-tunable bandgap, low-temperature solution processability. Lead sulfide (PbS) CQDs, with a strong absorption coefficient and large Bohr radius, enable solar cells to harvest infrared photons of the solar spectrum beyond the absorption edge of crystalline silicon and perovskites. There have been many strategies to improve device performance, among which interface engineering is a promising method. Excellent interface engineering is designed to form an energy cascade to enable an efficient charge transfer and promote exciton dissociation. Moreover, it can also offer good interfacial contact and improve device air stability by selecting appropriate materials. Here, we use phenyl-C61-butyric acid methyl ester (PCBM) as the interlayer between QDs and electron transport layer, and additive into PbS CQD solution to fabricate PbS QD solar cells and study the trap densities and charge transport process at QDs interfaces.

CPP 8.17 Wed 17:30 P

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-Frank-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 tailored nanostructures on the film surface are detected by surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by GISAXS.

CPP 8.18 Wed 17:30 P

Sol-gel based tailored lithium-ion battery electrodes — ●IVANA PIVARNÍKOVÁ^{1,2}, RALPH GILLES¹, and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — ²Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

Silicon (Si) based materials have been considered one of the most promising candidates for the next-generation lithium-ion battery an-

odes. The aim of this work is the usage of copolymer assisted sol-gel synthesis of mesoporous silica thin films for anode application. This wet chemical method consists of the formation of the organic-inorganic composites by a self-assembly mechanism, where the organic phase (PEO-*b*-PPO-*b*-PEO non-ionic triblock copolymer) serves as a template for the inorganic structure (SiO₂). The tetraethoxysilane (TEOS) is used as a Si precursor. The solution mix is coated onto the cleaned Si substrates and the template removal is done by calcination at high temperature (400 °C). The properties of the thin films can be tuned by adjusting the synthesis conditions such as concentration of reaction compounds, choice of the deposition technique or choice of the final calcination step. The aim is to reach the desired thickness, porosity, conductivity and mechanical stability for the successful Li-ion battery anode application. Thin films are characterized by scanning electron microscopy (SEM), grazing incidence small-angle X-ray scattering (GISAXS), profilometry and ellipsometry measurements.

CPP 8.19 Wed 17:30 P

The influence of toluene in an Si/Ge sol-gel approach — ●CHRISTIAN L. WEINDL¹, CHRISTIAN FAJMAN², MICHAEL A. GIEBEL², MATTHIAS SCHWARZKOPF³, STEPHAN V. ROTH^{3,4}, THOMAS F. FÄSSLER², and PETER MÜLLER-BUSCHBAUM^{1,5} — ¹Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ²Lehrstuhl für Anorganische Chemie mit Schwerpunkt Neue Materialien, Chemie Department, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — ³Deutsches Elektronen-Synchrotron DESY, Notkestr.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 (LIBs). Owing to their high energy capacity these two group 14 semiconductors are considered as auspicious alternatives to graphite anodes in LIBs. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a well-known wet chemical sol-gel approach. Here, the amphiphilic diblock copolymer polystyrene-block-polyethylene oxide (PS-*b*-PEO) is used as the structuring agent. In the experiment, we investigate the structural difference that occurs when toluene is used as an additive. Real-space data as SEM and EDX spectroscopy will be discussed with reciprocal-space analysis methods as GISAXS.

CPP 8.20 Wed 17:30 P

Investigation of Au(100) and Au(110) surfaces in electrolyte by Reflection Anisotropy Spectroscopy (RAS) — ●MARIO LÖW¹, MARGOT GUIDAT¹, TIMOTHÉE GÔMES^{1,2}, JONGMIN KIM¹, and MATTHIAS M. MAY¹ — ¹Ulm University, Institute of Theoretical Chemistry, D-89081 Ulm — ²Chimie Paristech - PSL, F-75005 Paris

Rechargeable magnesium batteries will probably play a huge role in the future of the battery market. However, there is until now no standard cathode material, like for lithium ion batteries. One possible material could be the porphyrin molecule CuDEPP.[1]

To get a deeper knowledge on how the structure of this molecule changes while applying a voltage, its adsorption on the well-ordered Au-surfaces is studied by Reflection Anisotropy Spectroscopy (RAS). This technique allows to investigate the structure of the interface while applying potentials in the electrolyte.

As a starting point for this investigation, we first establish the surface of the well-ordered Au-surface with RAS (in electrolyte) as a reference. Then we relate this spectra to electronic structure models via computational spectroscopy to understand chemical and physical processes that occur at the electrochemical double layer. Here, we show first results employing the approach.

[1] Abouzari-Lotf, Ebrahim, et al. ChemSusChem 14.8 (2021): 1840-1846.

CPP 8.21 Wed 17:30 P

Tuning the electronic and magnetic properties of graphene with periodically arranged metal-organic coordination networks — ●QIANKUN WANG, BRIAN D. BAKER CORTÉS, JORIS DE LA RIE, MIHAELA ENACHE, and MEIKE STÖHR — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Here, we investigated by means of scanning tunneling microscopy and photoelectron spectroscopy how the electronic properties of graphene are modified upon deposition of 5,10,15,20-tetra(4-pyridyl)porphyrin

(H2TPyP) with and without coordination to Co atoms. Graphene was prepared on Cu(111) via chemical vapor deposition, and it is known to be n-type doped. We will discuss (i) the transition of the H-bonded self-assembled H2TPyP network into a long-range ordered metal-organic coordination network (MOCN) upon Co deposition and (ii) the electronic level alignment at the graphene/MOCN interface and how this is influenced by the underlying substrate. Our study provides a viable possibility for the usage of graphene as a charge and spin transport material in future electronic and spintronic applications.

CPP 8.22 Wed 17:30 P

bias- and concentration-dependent switching of supramolecular nanostructures at the solid-liquid interface — ●BAOXIN JIA¹, MIHAELA ENACHE¹, SANDRA MIGUEZ-LAGO², MILAN KIVALA², and MEIKE STÖHR¹ — ¹Zernike Institute for Advanced Materials, University of Groningen, Netherlands — ²Institute of Organic Chemistry, University of Heidelberg, Germany

Research into the controlled switching between different molecular phases at the solid-liquid interface induced by an external electric field has gained increasing attention over the past years. Here we discuss the bias- and concentration-dependent switching of a carboxy-functionalized triarylamine derivative at the nonanoic-HOPG interface studied by scanning tunneling microscopy. For a fully saturated solution, a porous phase (chickenwire) was observed for negative sample bias and a close-packed phase for positive sample bias. For a 50% saturated solution, a second porous phase (flower) coexisted with the chickenwire phase at negative sample bias, while the close-packed phase was still observed at positive sample bias. For a 20% saturated solution, the two porous phases and the close-packed phase coexisted at positive sample bias because of the low molecule concentration in the solution, while the two porous phases were observed at negative bias. For all concentrations investigated, by changing the polarity of bias voltage, a reversible phase transformation between the porous phases to the close-packed phase was accomplished. Our study demonstrates that controlled structural changes can be accomplished by changing the polarity of the applied external field.

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Phase Transitions in Disordered Mesoporous Solids: Effect of Geometric Disorder — ●HENRY R. N. B. ENNINFUL, DIRK ENKE, and RUSTEM VALIULLIN — Leipzig University, Leipzig, Germany

Majority of porous solids used in industrial processes such as energy storage, separations and catalysis possess structural disorder over varying length scales. These disorder effects strongly affect the properties of the confining fluids in the pores. Hence, detailed quantification of structural disorder with correlation to fluid phase behavior is a necessary step towards optimization for practical applications.

Employing the serially connected pore model, (SCPM), we have determined the impact of a number of disorder-related parameters, including effect of pore chain length, *powder effect* and interconnectivity effect on phase transitions in disordered mesopore spaces. Additionally, we have showed experimental results from solid-liquid phase transitions obtained by NMR cryoporometry and gas-liquid transitions observed from nitrogen sorption experiments to corroborate the theoretical predictions from the SCPM.

We conclude that, the SCPM has the potential of explaining many features of experimentally observed phase transitions in disordered mesoporous solids.

References [1] Enniful et 2020, Microporous and Mesoporous Materials 309, 110534. [2] Enniful et 2021, Langmuir 37, 12, 3521*3537.

CPP 8.24 Wed 17:30 P

Real-time observations of alkali metal doped 6-Phenacene films — ●MATTHIAS ZWADLO¹, JAKUB HAGARA², GIULIANO DUVA¹, JAN HAGENLOCHER¹, ALEXANDER GERLACH¹, MARTIN HODAS¹, ALEXANDER HINDERHOFER¹, PETER SIFFALOVIC², and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²Institute of Physics, Slovak Academy of Sciences Bratislava, Slovakia

The characterization of growth and structure formation in molecular und hybrid e.g. doped systems is an important topic in fundamental organic semiconductor research. In order to study and influence this process different real-time methods have to be used [1]. The growth and structure formation of pure 6-Phenacene as well as the effects of potassium, caesium and rubidium doping were investigated. Thin films of pure 6-Phenacene have been grown in ultra-high vacuum (UHV) and investigated with x-ray, AFM and optical methods. Furthermore,

in-situ GIWAXS measurements were performed at PETRA 3 P03. Results on 6-Phenacene as well as preliminary doping results have been published [2]. Doping shows small distortions in crystal structure as well as optical spectra which are yet under investigation and will allow us to get a better understanding on the structural behavior and growth process in theory and experiment.

[1] Hosokai, T., et al., Appl. Phys. Lett., 97(6), 9 (2010) doi:10.1063/1.3478450

[2] Zwadlo, M., et al., Adv. Optical Mater. (2021), 9, 2002193. doi:/10.1002/adom.202002193

CPP 8.25 Wed 17:30 P

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 GALLET⁴, 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) 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 inside a closed chamber 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 8.26 Wed 17:30 P

Influence of Chaotropic NaBr on the Swelling Behavior of PNIPMAM Thin Films — •JULIA REITENBACH¹, CHRISTINA GEIGER¹, PEIXI WANG¹, LUCAS P. KREUZER¹, ROBERT CUBITT², VIET HILDEBRAND³, ANDRÉ LASCHEWSKY³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France — ³Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

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 polymers 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.

CPP 8.27 Wed 17:30 P

Made2Reflect: A tool for joint analysis of neutron reflectometry data and Molecular Dynamics Simulations of interfaces — •NEBOJŠA ZEC¹, GAETANO MANGIAPIA¹, HANH VI LÊ², MURIEL ROVIRA ESTEVA¹, SEBASTIAN BUSCH¹, and JEAN-FRANÇOIS MOULIN¹ — ¹German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ) Helmholtz-Zentrum Hereon Lichtenbergstr. 1, 85747 Garching bei München, Germany — ²SMIS beamline, synchrotron Soleil, L'orme des Merisiers Saint-Aubin, BP 48 91192 Gif-sur-Yvette Cedex

Neutron and X-Ray reflectometry are standard methods for the investigation of thin films and interfaces. Data inversion leading to a structural model is rendered difficult by the well known phase problem. Molecular Dynamics Simulations (MD) are another tool used to study interfaces. MD however has problems of its own: convergence

issues and validity of the force fields, to name a few. We show here how jointly using MD and reflectometry can help elucidate details of interfacial structures such as those typically encountered in cell membranes, thin polymer films or electrochemistry. We have developed a Python software tool (Made2Reflect) which makes it easy to extract a scattering length density profile from atomistic MD and compute the corresponding reflectivity curve, thereby taking into account all aspects of the sample as well as the experimental effects such as the instrumental resolution. Actual examples will be shown illustrating that this joint method allows to (in)validate structural hypotheses which cannot be tested by means of any one of the techniques used alone.

CPP 8.28 Wed 17:30 P

Fabricating high resolution nanostructures using polymethyl methacrylate and isopropanol water mixtures — •STEPHANIE LAKE¹, FRANK HEYROTH², and GEORG SCHMIDT^{1,2} — ¹Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — ²Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Electron beam lithography (EBL) can produce high resolution structures but has its drawbacks. Compared to photolithography, it takes more time and has lower throughput. An ideal EBL procedure would require lower exposure dose and withstand environmental fluctuations. Establishing a "process window" (PW) quantifies such requirements.

In this poster, we define a primary PW for polymethyl methacrylate (PMMA) during the developer stage. The area dose is varied and the range where there is sufficient development is subsequently identified. Isopropanol (IPA) and water mixtures can decrease the exposure dose needed for full development compared to other standard PMMA developers¹. Thus, we defined yet another PW by varying the IPA concentration and measuring the aforementioned, primary PW.

From this work, we discovered mixtures of 69% to 77% IPA can require lower exposure doses than pure IPA. With 73% IPA, the required dose can be up to 82.9% less than that for pure IPA. We show it is feasible to use this developer for high resolution structures without compromising reproducibility.

¹Mohsin, M. A. & Cowie, J. M. G. *Polymer (Guildf)*. **29**, 2130-2135 (1988).

CPP 8.29 Wed 17:30 P

A thermoresponsive poly(2-oxazoline)-based molecular brush in aqueous solution: effect of a cosolvent — •BAHAR YAZDANSHENAS¹, CLEMENS SACHSE², STEFANO DA VELA³, RAINER JORDAN², and CHRISTINE M. PAPADAKIS¹ — ¹Technische Universität München, Physik-Department, Garching, Germany — ²Technische Universität Dresden, Fakultät Chemie und Lebensmittelchemie, Dresden, Germany — ³EMBL c/o DESY, Hamburg, Germany

Poly(2-oxazoline)s are well-known for their easy and direct synthesis, providing access to well-defined structures, with tunable properties [1]. In this study, a 1 wt% PiPOx₁₀₀-g-PETox₁₇ molecular brush with a poly(2-isopropenyl-2-oxazoline) (PiPOx) thermoresponsive backbone grafted with thermoresponsive poly(2-ethyl-2-oxazoline) (PETox) side chains is investigated in water-ethanol solvent mixtures. This densely grafted polymer with functional and biocompatible segments can be attractive for many applications, such as biomaterials.

In aqueous solution of 3 wt% of this molecular brush, lower critical solution temperature (LCST) behavior has been observed with an increase of the brush length upon heating from room temperature to T_{cp} [2]. In water-ethanol solvent mixtures of 1 wt% concentration, T_{cp} increases with the ethanol fraction. The temperature-dependent structural evolution is investigated using dynamic light scattering and synchrotron small-angle X-ray scattering.

[1] R. Hoogenboom, *Angewandte Chemie International Edition*, 2009, 48, 7978 [2] J.-J. Kang, C. M. Papadakis et al., *Colloid Polym. Sci.* 2021, 299, 193

CPP 8.30 Wed 17:30 P

Highly Metastable Switchable Surfaces Based on Polymer Brushes Containing End-Adsorbing Chains — •MARKUS KOCH¹, DIRK ROMEIS¹, and JENS-UWE SOMMER^{1,2} — ¹Institute Theory of Polymers, IPF Dresden, Germany — ²Institute Theory of Physics, TU Dresden, Germany

We investigate a switchable polymer brush system that responds to external stimuli by adsorbing (hiding) or exposing specific functional groups. Our design enables targeted changes to the properties of a surface, e.g. to change the interactions with the environment or increase the density of functional groups below the brush. The system con-

sists of a monodisperse polymer brush containing a small fraction of end-modified minority chains. The length of these chains differs from the brush and their end groups can adsorb at the grafting surface. We study this system using Scheutjens-Fleer SCF calculations, MD simulations, and analytical theory [1]. The conformational changes of the admixed chains depend on their relative length and the attraction of their end groups to the surface. Based on the free energy profiles of the adsorption transition, we extract free energy barriers, that are in good agreement with our theoretical predictions. The barriers are strongly reduced when the brush is collapsed, for instance, via a solvent change. Thus, the system can be tuned to obtain a reversible or irreversible end-adsorption behavior. Financial support by the DFG, project SO 277/17-1, is gratefully acknowledged.

[1] Koch, M., Romeis, D., Sommer, J.-U., *Macromolecules* 53 (17), 7356-7368 (2020)

CPP 8.31 Wed 17:30 P

Effect of pressure on the micellar structures of PMMA-b-PNIPAM in aqueous solution — ●PABLO A. ÁLVAREZ HERRERA¹, GEETHU P. MELEDAM¹, CHIA-HSIN KO¹, BART-JAN NIEBUUR¹, SHU-HSIEN HUANG¹, LEONARDO CHIAPPISI², CRISTIANE HENSCHL³, ANDRÉ LASCHEWSKY³, ALFONS SCHULTE⁴, and CHRISTINE M. PAPADAKIS¹ — ¹TU München, Physik-Department, Garching, Germany — ²Institut Laue-Langevin, Grenoble, France — ³Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — ⁴University of Central Florida, Orlando, USA

Amphiphilic diblock copolymers feature self-assembly behavior in aqueous solution. In particular, poly(methyl methacrylate)-b-poly(N-isopropylacrylamide) (PMMA-b-PNIPAM) forms core-shell micelles upon heating above the cloud point (T_{CP}). In aqueous solutions of PNIPAM homopolymers, it was previously found that the dehydra-

tion behavior is strongly altered by pressure [1]. We study the effect of pressure on the micellar structure of PMMA-b-PNIPAM in aqueous solution by small-angle neutron scattering (SANS). In temperature-resolved experiments at 0.1 and 75 MPa, we find that the micelles dehydrate and collapse above T_{CP} at low pressure, while the PNIPAM shells remain hydrated, and the micelles form large clusters at higher pressure.

I.B.-J. Niebuur, C. M. Papadakis et al., *ACS Macro Lett.* 2017, 6, 1180 and *Macromolecules* 2019, 52, 1942.

CPP 8.32 Wed 17:30 P

Co-nonsolvency behavior of responsive polymers in thin film/vapor systems — ●CHRISTINA GEIGER¹, MORGAN LE DÛ¹, ANNA LENA OECHSLE¹, PEIXI WANG¹, SUO TU¹, ROBERT CUBITT², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²Institut Laue-Langevin, 38000 Grenoble, France

After exposure to mixed water/cosolvent vapor, hydrated thin films of stimuli-responsive block copolymers with PNIPAM or PNIPMAM blocks exhibit a co-nonsolvency behavior. In a rapid film contraction, in either system, both water and cosolvent are expelled. Film swelling and contraction kinetics from saturated vapor are investigated in time-of-flight neutron reflectometry (ToF-NR) with simultaneous spectral reflectance (SR). Molecular interactions of the solvent with the respective polymer chains are analyzed with Fourier-transform infrared (FTIR) spectroscopy. In our latest study with PNIPAM, we focus on the swelling behavior in mixed vapors starting not from the hydrated, but from the dry film state. A minimum in reached thickness due to the co-nonsolvency effect is found, which is reversely related to the interaction strength of polymer chains facilitated by the present water/cosolvent ratio.