

## Chemical and Polymer Physics Division Fachverband Chemische Physik und Polymerphysik (CPP)

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### Overview of Invited Talks and Sessions

(Lecture halls CPPa, and CPPb; Poster CPPp)

#### Invited Talks

CPP 2.6	Mon	11:00–11:40	CPPa	<b>Singlet fission in blends of organic semiconductors</b> — •KATHARINA BROCH, CLEMENS ZEISER, LUCA MORETTI, CHAD CRUZ, GIULIO CERULLO, ROEL TEMPELAAR, CHRISTOPHER BARDEEN
CPP 2.11	Mon	14:00–14:40	CPPa	<b>Small, but highly effective: Functional molecules in polymer devices</b> — •ULRIKE KRAFT
CPP 3.5	Mon	11:00–11:40	CPPb	<b>Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates</b> — •RALF SEEMANN, ROGHAYEH SHIRI, STEFAN BOMMER, DIRK PESCHKA, SEBASTIAN JACHALSKI, LENOIE SCHMELLER, BARBARA WAGNER
CPP 3.10	Mon	14:00–14:40	CPPb	<b>Sinking droplet durotaxis and engulfment</b> — •ANNE JUEL
CPP 7.5	Tue	11:00–11:40	CPPa	<b>Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites</b> — •FELIX DESCHLER
CPP 7.9	Tue	14:00–14:40	CPPa	<b>Structural dynamics of halide perovskites via in-situ electron microscopy</b> — •CHEN LI
CPP 8.1	Tue	9:00– 9:40	CPPb	<b>Polymer Micelles with Crystalline Cores: confinement effects, molecular exchange kinetics and mechanical response</b> — NICO KOENIG, LUTZ WILLNER, •REIDAR LUND
CPP 8.4	Tue	11:00–11:40	CPPb	<b>Dynamic behaviour of anisotropic magnetic particles in suspensions</b> — •SOFIA KANTOROVICH
CPP 16.1	Wed	9:00– 9:40	CPPa	<b>Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors</b> — •CHRISTIAN HOLM, KONRAD BREITSPRECHER, SVY-ATOSLAV KONDRAT
CPP 16.4	Wed	11:00–11:40	CPPa	<b>Interaction of polyelectrolytes with proteins</b> — •MATTHIAS BALLAUFF
CPP 17.1	Wed	9:00– 9:40	CPPb	<b>Data-driven methods in polymer physics: exploring the sequence space of copolymers</b> — •MARCO WERNER
CPP 17.6	Wed	11:40–12:20	CPPb	<b>Structure formation in drying films and droplets</b> — •ARASH NIKOUBASHMAN, MICHAEL HOWARD, MICHAEL KAPPL, HANS-JÜRGEN BUTT

#### Sessions

CPP 1	Mon	8:50– 9:00	CPPa	<b>Welcome</b>
CPP 2.1–2.15	Mon	9:00–16:30	CPPa	<b>Molecular Electronics - organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)</b>
CPP 3.1–3.14	Mon	9:00–16:30	CPPb	<b>Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)</b>
CPP 4.1–4.4	Mon	9:00–11:00	BPb	<b>Active Biological Matter I (joint session BP/DY/ CPP)</b>
CPP 5.1–5.6	Mon	11:00–13:30	BPb	<b>Active Biological Matter II (joint session BP/ CPP/DY)</b>
CPP 6.1–6.17	Mon	16:30–18:30	CPPp	<b>Poster Session I - Molecular Electronics and Wetting</b>
CPP 7.1–7.12	Tue	9:00–16:30	CPPa	<b>Perovskites - organized by Eva M. Herzig (University of Bayreuth, Bayreuth)</b>

CPP 8.1–8.13	Tue	9:00–16:30	CPPb	<b>Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)</b>
CPP 9.1–9.4	Tue	9:00–11:00	BPc	<b>Focus Phase Separation in Biological Systems I (joint session BP/ CPP)</b>
CPP 10.1–10.3	Tue	9:30–10:30	DYa	<b>Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/ CPP)</b>
CPP 11.1–11.6	Tue	11:00–13:00	DYa	<b>Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/ CPP)</b>
CPP 12.1–12.4	Tue	14:00–16:00	BPb	<b>Focus Phase Separation in Biological Systems II (joint session BP/ CPP)</b>
CPP 13.1–13.6	Tue	14:30–16:30	DYc	<b>Complex Fluids and Soft Matter 3 (joint session DY/ CPP)</b>
CPP 14.1–14.26	Tue	16:30–18:30	CPPp	<b>Poster Session II - Complex Fluids and Perovskites</b>
CPP 15	Tue	17:45–18:30	BPb	<b>Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/ CPP/ DY/ SOE)</b>
CPP 16.1–16.12	Wed	9:00–15:20	CPPa	<b>Charged Soft Matter - organized by Joachim Dzubiella (Albert Ludwigs University Freiburg, Freiburg)</b>
CPP 17.1–17.10	Wed	9:00–14:40	CPPb	<b>Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/ DY)</b>
CPP 18.1–18.4	Wed	9:00–10:30	DYa	<b>Complex Fluids and Soft Matter 1 (joint session DY/ CPP)</b>
CPP 19.1–19.3	Wed	9:30–10:30	DYc	<b>Glasses and Glass Transition 1 (joint session DY/ CPP)</b>
CPP 20.1–20.6	Wed	11:00–13:00	DYa	<b>Complex Fluids and Soft Matter 2 (joint session DY/ CPP)</b>
CPP 21.1–21.6	Wed	11:00–13:00	DYc	<b>Glasses and Glass Transition 2 (joint session DY/ CPP)</b>
CPP 22.1–22.43	Wed	16:30–18:30	CPPp	<b>Poster Session III - Charged Soft Matter and Theory and Simulation</b>

## CPP 1: Welcome

Time: Monday 8:50–9:00

Location: CPPa

Welcome

## CPP 2: Molecular Electronics - organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)

Time: Monday 9:00–16:30

Location: CPPa

CPP 2.1 Mon 9:00 CPPa

**Organic light-emitting diodes for high-brightness operation: self-heating and switched-back regions** — ●ANTON KIRCH<sup>1</sup>, AXEL FISCHER<sup>1</sup>, MATTHIAS LIERO<sup>2</sup>, JÜRGEN FUHRMANN<sup>2</sup>, ANNEGRET GLITZKY<sup>2</sup>, and SEBASTIAN REINEKE<sup>1</sup> — <sup>1</sup>Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany — <sup>2</sup>Weierstrass Institute Berlin, Germany

Nonlinear effects typically involve switching phenomena that can lead to abrupt catastrophic device failure. For example, organic light-emitting diodes (OLEDs) suffer from strong electrothermal feedback that arises upon Joule self-heating. The interaction between temperature-dependent conductivity and power dissipation results in a positive feedback loop that finally destroys the device by thermal runaway. The situation becomes more severe for large-area OLEDs where the operation regime can locally differ. Former modeling studies, using a network of thermistors, led to the proposal that a so-called \*switched-back\* region arises. In this area, the current density, as well as the brightness, decreases although the total device current still increases when running an IV scan.

Here, we experimentally prove the existence of a switched-back region. We demonstrate that its appearance agrees with the simulation that solely uses electrothermal modeling. Our study aims to improve the long-term stability of high brightness OLED lighting tiles e.g. as applied in the automotive sector.

CPP 2.2 Mon 9:20 CPPa

**Numerical Modeling of Transient Electroluminescence based on Thermally Activated Delayed Fluorescence** — ●JEANNINE GRÜNE, NIKOLAI BUNZMANN, SEBASTIAN WEISSENSEEL, VLADIMIR DYAKONOV, and ANDREAS SPERLICH — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) show increased efficiencies due to effective upconversion from the non-emissive triplet states to the emissive singlet state via reverse intersystem crossing (RISC). A promising approach in this field are donor:acceptor configurations, whereby an intermolecular exciton is formed at the interface of two molecules, also called exciplex. A proven material combination is among others 4,4',4''-Tris[(3-methylphenyl)phenylamino]triphenylamine (m-MTDATA), as donor and Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB), as acceptor. The characteristic behaviour especially in transient measurements differs from what is commonly observed in state of the art intramolecular emitters. In order to gain insight into the ongoing processes in exciplex based OLEDs, we performed numerical fits on transient electroluminescence (trEL) measurements at different temperatures. The kinetic model adapted for EL measurements on TADF systems includes second order terms to consider the existing annihilation processes such as triplet-triplet annihilation. Using this procedure, we can quantify the impact of efficiency-enhancing and efficiency-reducing processes as well as the time-dependent excited state populations.

CPP 2.3 Mon 9:40 CPPa

**Two-dimensional electronic spectroscopy of phthalocyanine on rare gas clusters** — ●ULRICH BANGERT, LUKAS BRUDER, MARCEL BINZ, FRIEDEMANN LANDMESSER, ELENA LEISLER, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

With the recent advances of two-dimensional electronic spectroscopy (2DES) towards the gas phase, versatile samples like rare gas cluster beams become accessible [1]. Doping rare gas clusters with multiple molecules yields well defined many body systems. These systems are comparable to highly dilute thin film, however feature weak interaction

with the substrate and are cooled down to  $\leq 10$  K. In previous experiments, such systems provided valuable details about singlet fission and super radiance in acene molecules [2,3]. We now apply for the first time 2DES to this approach and study free-base phthalocyanine in different environments: embedded in superfluid helium nanodroplets, deposited on the surface of neon clusters and as a thermal vapor. We find distinct differences in the photodynamics of the molecular assemblies.

[1] L. Bruder et al., J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).

[2] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).

[3] M. Müller et al., Phys. Rev. B 92 (12), 121408 (2015).

CPP 2.4 Mon 10:00 CPPa

**Clarifying the orientation mechanism of homoleptic Iridium-carbene complexes** — ●MARKUS SCHMID<sup>1</sup>, KRISTOFFER HARMS<sup>2</sup>, THOMAS MORGENSTERN<sup>1</sup>, ALEXANDER HOFMANN<sup>1</sup>, HANS-HERMANN JOHANNES<sup>2</sup>, WOLFGANG KOWALSKY<sup>2</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Institute for high frequency technology, TU Braunschweig, 38106 Braunschweig, Germany

Horizontal orientation of the emitting species is one of the most promising techniques to increase the efficiency of state of the art organic light emitting diodes. Especially metal-organic compounds have attracted great attention. While the alignment has been observed and explained for many heteroleptic Iridium complexes, there has been less progress for their homoleptic counterparts. Only few homoleptic compounds have been reported to show a beneficial morphology in guest-host systems. In this study, we investigated multiple derivatives and isomers of the sky-blue dye tris(N-dibenzofuranyl-N'-methylimidazole)iridium(III) (Ir(dbfmi)<sub>3</sub>) doped in the hosts Bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) and 3,6-bis(diphenylphosphoryl)-9-phenylcarbazole (PO9). By a combination of optical techniques to probe the transition dipole orientation and electrical measurements to access the permanent dipole moment, we revealed that this homoleptic complex is significantly aligned in both matrices. From our insights into the film morphology we postulate that an anisotropic interaction is responsible for the orientation and even identified the region of the molecule that causes this behavior.

CPP 2.5 Mon 10:20 CPPa

**Understanding Ultrafast Proton Transfer in Molecular Crystals** — ●HYEIN HWANG<sup>1,2</sup>, VANDANA TIWARI<sup>3</sup>, SIMON /F. BITTMANN<sup>1</sup>, HONG-GUANG DUAN<sup>4</sup>, FRIEDJOF TELLKAMP<sup>1</sup>, AJAY JHA<sup>5</sup>, and R. J. DWAYNE MILLER<sup>6</sup> — <sup>1</sup>Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — <sup>2</sup>Department of Chemistry, University of Hamburg, Germany — <sup>3</sup>European XFEL, Hamburg, Germany — <sup>4</sup>Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — <sup>5</sup>RFI, Harwell Oxford, United Kingdom — <sup>6</sup>Department of Chemistry, University of Toronto, Ontario, Canada

Ultrafast proton transfer reaction is a topic of great interest particularly due to their association with the understanding of primary and elementary reaction pathways in functional electrochemical and biological systems. Although this reaction has been extensively investigated in solution for the role of interaction between the solute and the solvent-bath, but the dynamics in single molecular crystals remains elusive. Here, we study ultrafast intramolecular proton transfer reaction in hydroxyanthraquinones in crystalline form, where molecular system forms lattice. We use ultrafast transient absorption studies complemented with quantum chemistry calculations to reveal the role of spatial arrangement of the reactants within the lattice in reaction dynamics. Our work highlight the importance of intermolecular interactions guiding ultrafast dynamics in crystals.

## 20 min. meet the speakers - break

## Invited Talk

CPP 2.6 Mon 11:00 CPPa

**Singlet fission in blends of organic semiconductors** — ●KATHARINA BROCH<sup>1</sup>, CLEMENS ZEISER<sup>1</sup>, LUCA MORETTI<sup>2</sup>, CHAD CRUZ<sup>3</sup>, GIULIO CERULLO<sup>2</sup>, ROEL TEMPELAAR<sup>4</sup>, and CHRISTOPHER BARDEEN<sup>3</sup> — <sup>1</sup>Institute for Applied Physics, University of Tübingen, Germany — <sup>2</sup>Department of Physics, Polytechnic University of Milan, Italy — <sup>3</sup>Department of Chemistry, University of California at Riverside, USA — <sup>4</sup>Department of Chemistry, Northwestern University, USA

Singlet fission (SF), the photophysical process converting an singlet state into two triplets, is a promising approach to boost solar cell efficiencies [1], and is, due to a triplet-pair state intermediate, also interesting from the viewpoint of fundamental research. SF rates are controlled by the interplay of intermolecular interactions, energetics and electron-phonon coupling and a controlled modification of these parameters is key to a fundamental understanding of this complex process. Blends of organic semiconductors present an interesting alternative to established methods of chemical functionalization [2,3] and their potential for the study and control of SF pathways will be discussed using two examples of acene blends [3,4].

[1] M. B. Smith, J. Michl, *Annu. Rev. Phys. Chem.* 64 (2013); [2] D. Lubert-Perquel et al., *Nat. Commun.* 9 (2018); [3] K. Broch et al., *Nat. Commun.* 9 (2018); [4] C. Zeiser et al., *Angew. Chem. Int. Ed.* 59 (2020)

CPP 2.7 Mon 11:40 CPPa

**Influence of alkyl chain variation on co-crystal formation and molecular charge transfer** — ●NADINE RUSSEGER, OLEG VLADIMIROV, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground state and in the excited state.

In this work, the charge transfer effect of weakly interacting organic semiconductor mixtures is comprehensively investigated depending on the influence of alkyl chain variation with different acceptor molecules. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNFT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different alkyl chain length in the imide position as acceptor molecules (PDIF-CN<sub>2</sub>, PDI-C3, PDI-C5, and PDI-C8-CN<sub>2</sub>).

For a full structural overview of the resulting molecularly mixed co-crystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption, photoluminescence as well as *in-situ* differential reflectance spectroscopy. For the various equimolar mixed systems of DNFT as well as DIP and different perylene-diimide derivatives charge transfer effects were estimated [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the chain length and their configuration of the different mixed systems.

[1] V. Belova et al., *J. Am. Chem. Soc.*, 2017, 139, 8474-8486.

CPP 2.8 Mon 12:00 CPPa

**Anisotropic Charge Transfer Formation at Crystalline Pentacene/Perfluoropentacene Interfaces** — ●SEBASTIAN HAMMER<sup>1</sup>, CLEMENS ZEISER<sup>2</sup>, KATHARINA BROCH<sup>2</sup>, and JENS PFLAUM<sup>1,3</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Institute for Applied Physics, University of Tübingen, 72076 Tübingen — <sup>3</sup>ZAE Bayern, 97074 Würzburg

Strongly bound charge transfer (CT) states critically influence the performance of devices based on donor/acceptor (D/A) heterojunctions such as light emitting diodes or photovoltaic cells. Whereas the excited states in the archetypical CT system Pentacene:Perfluoropentacene (P:PFP) have been vastly studied in thin films [1][2], the role of molecular orientation on CT formation and energetics has not been evaluated to the same extent, so far. Utilizing heteroepitaxial growth of PFP on P (001) single crystals surfaces we were able to prepare long-range ordered D/A heterojunctions in an edge-on molecular configuration as confirmed by XRD. Optical analyses by temperature dependent cw-fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy on the PFP/P interfaces revealed no indication for CT formation in case of edge-on molecular orientation, in contrast to the face-to-face geometry. By means of bilayer as well as heterojunction diode structures we demonstrate that by controlling the molecular orientation at the PFP/P interface, thus, utilizing the anisotropic CT

characteristics, the overall performance can be significantly improved.

[1] K. Broch et al., *Phys. Rev. B* 83, 245307 (2011)

[2] T. Breuer, G. Witte, *J. Chem. Phys.* 21, 138 (2013)

CPP 2.9 Mon 12:20 CPPa

**Ab initio modelling of local interfaces in doped organic semiconductors** — ●ANA MARIA VALENCIA, GUERRINI MICHELE, and CATERINA COCCHI — Humboldt-Universität zu Berlin

Despite the intensive efforts in the last decade, a clear and comprehensive understanding of the microscopic properties of doped organic semiconductors is still missing. Due to the complexity of these systems, which notoriously exhibit high level of disorder, also the results from quantum-mechanical ab initio methods are somehow constrained by the choice of the model structures. For a reliable prediction of electronic and optical properties, it is essential to rationalize the role of local interfaces between interacting donor and acceptor species. We address this problem from hybrid density-functional theory and many-body perturbation theory, investigating the structural, electronic, and optical properties of oligothiophenes doped by F4TCNQ. We consider different structures from isolated dimers and trimers, to periodic stacks and crystalline arrangements. Our results show that, depending on the amount and the nature of the local donor/acceptor interfaces, the choice of the simulated structure critically impacts the resulting electronic structure and degree of charge transfer. On the other hand, the optical spectra appear less sensitive to these characteristics, although a detailed inspection of the electron and hole densities discloses different excitation character depending on the relative donor/acceptor concentration [1] as well as on the donor length [2].

[1] Valencia, Guerrini, Cocchi, submitted (2019).

[2] Valencia & Cocchi, *JPCC* 123, 9617 (2019).

CPP 2.10 Mon 12:40 CPPa

**Impact of electron-phonon-interaction on transport in organic molecular crystals: Naphthalene as a case study** — ●KONRAD MERKEL, MICHEL PANHANS, SEBASTIAN HUTSCH, and FRANK ORTMANN — Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden

Understanding charge carrier transport in organic semiconductors is a key requirement for developing advanced electronic and opto-electronic devices such as OLEDs, OFETs and organic solar cells. However the general transport mechanism remains unclear. It is widely believed that electron-phonon-interaction plays an important role, due to the large fluctuations in the electronic coupling associated to the van-der-Waals-bonds between adjacent molecules. The interaction leads to a subtle interplay of scattering and phonon-assisted transport. Within the Kubo formalism, we derive a simulation technique, where we model the low-frequency phonon modes as local and non-local disorder in a tight-binding scheme and where all material parameters are calculated from density functional theory. We study the impact of such modes in naphthalene and compare our results to studies from literature.

## 60 min. meet the speakers - break

## Invited Talk

CPP 2.11 Mon 14:00 CPPa

**Small, but highly effective: Functional molecules in polymer devices** — ●ULRIKE KRAFT — Max Planck Institute for Polymer Research, Mainz, Germany

The incorporation of small functional molecules such as dopants, plasticisers or molecular switches into polymer films can strongly affect their properties and even induce additional functionalities. Here, two examples will be discussed in which small functional molecules significantly influence the (electronic) properties of polymer devices:

Firstly, intrinsically stretchable interconnects and electrodes are printed from conductive inks consisting of PEDOT:PSS and ionic additives. In this approach, the ionic additives act as dopants and plasticisers and film properties can be tuned by orders of magnitude.

Secondly, the bias stress stability of polymer transistor is significantly improved by the addition of specific functional molecules. While on-state bias stress stability is widely studied, the off-state bias stress is mostly overlooked, even though equally important. We close this gap, focus on the off-state bias stress stability and show that threshold voltage shifts can be remarkably reduced.

CPP 2.12 Mon 14:40 CPPa

**Single step production of a self-organized, low work function cathode interlayer from polymer blend solution** — ●DOMINIQUE

LUNGWITZ<sup>1</sup>, KELI FABIANA SEIDEL<sup>2</sup>, ANDREAS OPITZ<sup>1</sup>, THOMAS KRÜGER<sup>3</sup>, JAN BEHREND<sup>3</sup>, SETH R. MARDER<sup>4</sup>, and NORBERT KOCH<sup>1,5</sup> — <sup>1</sup>Institut für Physik and IRIS Adlershof, Humboldt Universität zu Berlin, Germany — <sup>2</sup>Physics Department, Universidade Tecnológica Federal do Paraná, Brasil — <sup>3</sup>Berlin Joint EPR Lab and Institut für Experimentalphysik, Freie Universität Berlin, Germany — <sup>4</sup>School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics (COPE), Georgia Institute of Technology Atlanta, USA — <sup>5</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Using cathode interlayers for reducing the work function of electrodes in organic electronic devices is a widely studied method. Here, we report a simple procedure to obtain a self-organized interlayer on ITO electrodes from a blend solution of P(NDI2OD-T2) and PEI. Reduced contact resistance and increased polymer conductivity are observed due to vertical phase separation. Fermi level pinning of P(NDI2OD-T2) at PEI covered ITO electrodes leads to the lowest possible electron injection barrier. Furthermore, an increased charge carrier density was measured. Finally, we relate the increase in polymer conductivity to a reduction of interfacial electron trapping and a morphology change. The results show clearly the importance of differentiation between work function reduction upon interfacial layers and conductivity increase upon changes of structural conformation.

CPP 2.13 Mon 15:00 CPPa

**Morphological investigations on fullerene-free bulk heterojunction blends for photovoltaic applications** — ●SEBASTIAN GROTT<sup>1</sup>, LORENZ BIESSMANN<sup>1</sup>, NITIN SAXENA<sup>1</sup>, WEI CAO<sup>1</sup>, SIGRID BERNSTORFF<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS funktionelle Materialien, 85748 Garching — <sup>2</sup>Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

In the last decades, the focus of research has been drawn towards the field of organic electronics due to their advantageous properties, such as versatility, flexibility, low-cost manufacturing processes, as well as their tuneable characteristics, such as solubility and absorption. These properties open up a wide range of applications, especially, in the field of photovoltaics. Hence, organic photovoltaics represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 10% have been reported and thus receive industrial attention for commercialization. We study the inner morphology of a low band gap, fullerene-free bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural information are correlated with current density voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

CPP 2.14 Mon 15:20 CPPa

**Fast Processing of Charge Transport Layers in Organic Solar Cells** — ●HARALD HOPPE<sup>1,2</sup>, SHAHIDUL ALAM<sup>1,2</sup>, AMAN ANAND<sup>1,2</sup>,

AURELIEN SOKENG DJOURMESSI<sup>1,2</sup>, JOSE PRINCE MADALAIMUTHU<sup>1,2</sup>, PETER FISCHER<sup>4</sup>, and ULRICH S. SCHUBERT<sup>1,2,3</sup> — <sup>1</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University, Jena, Germany — <sup>2</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University, Jena, Germany — <sup>3</sup>Jena Center for Soft Matter (JCSM), Friedrich Schiller University, Jena, Germany — <sup>4</sup>Faculty of Mechanical Engineering, Ilmenau University of Technology, Ilmenau, Germany

Charge transport layers (CTLs) are very important in organic solar cells to allow for an efficient and selective extraction of photogenerated charge carriers. Upon their optimization important photovoltaic parameters such as fill factors are being directly affected, for example since the series resistance and parallel resistance are often improved in combination with each other, when the contact becomes more selective. Unfortunately, CTLs often require an additional and rather intensive annealing process, which will add to the energy investment to such solar cells. In addition, such annealing processes may often either require too high temperatures to be compatible with flexible substrates or may be too time-consuming for fast web speeds. As one solution, we demonstrate the successful application of flash sintering for the annealing of CTLs.

CPP 2.15 Mon 15:40 CPPa

**Polarized blue photoluminescence of mesoscopically ordered electrospun non-conjugated polyacrylonitrile nanofibers** — XIAOJIAN LIAO<sup>1</sup>, ●FRANK-JULIAN KAHLE<sup>2</sup>, BIN LIU<sup>3,4</sup>, HEINZ BÄSSLER<sup>2</sup>, XINGHONG ZHANG<sup>3</sup>, SEEMA AGARWAL<sup>1</sup>, ANNA KÖHLER<sup>2</sup>, and ANDREAS GREINER<sup>1</sup> — <sup>1</sup>Macromolecular Chemistry II, U Bayreuth, Germany — <sup>2</sup>Softmatter Optoelectronics, U Bayreuth, Germany — <sup>3</sup>MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Zhejiang University, P. R. China — <sup>4</sup>School of Energy and Power Engineering, North University of China, China

We demonstrate the fabrication of electrospun fibers from the non-conjugated polymer polyacrylonitrile (PAN) that can be aligned by a simple heat-stretching process. Upon excitation at 340 nm ribbons made from the nanofibers show polarized deep blue luminescence with an anisotropy of 0.37 and a quantum yield of about 0.31. Furthermore, they exhibit room temperature green phosphorescences with a lifetime of about 200 ms as well as a delayed deep blue fluorescence resulting from triplet-triplet annihilation (non-coherent photon upconversion). Wide and small angle X-ray scattering experiments show that the stretched electrospun nanofibers are highly aligned with nearly perfect uniaxial orientation within the fabricated ribbons. This results in mechanical robustness and flexibility, with a high specific tensile strength ( $534 \pm 28$ ) MPa · cm<sup>3</sup>/g and toughness ( $79 \pm 7$ ) J/g. The combination of efficient polarized deep blue luminescence, room temperature phosphorescence, TTA, mechanical robustness and flexibility of these fibers opens up new avenues for applications.

30 min. meet the speakers - break

### CPP 3: Wetting - organized by Stefan Karpitschka (Max Planck Institute for Dynamics and Self-Organization, Göttingen) (joint session CPP/DY)

Time: Monday 9:00–16:30

Location: CPPb

CPP 3.1 Mon 9:00 CPPb

**Breakup Dynamics of Capillary Bridges on Hydrophobic Stripes** — MAXIMILIAN HARTMANN<sup>1</sup>, ●MATHIS FRICKE<sup>2</sup>, LUKAS WEIMAR<sup>1</sup>, DIRK GRÜNDING<sup>2</sup>, TOMISLAV MARIC<sup>2</sup>, DIETER BOTHE<sup>2</sup>, and STEFFEN HARDT<sup>1</sup> — <sup>1</sup>Nano- and Microfluidics Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany — <sup>2</sup>Mathematical Modeling and Analysis Group, TU Darmstadt, Alarich-Weiss-Straße 10, 64287 Darmstadt, Germany

The breakup dynamics of a capillary bridge on a hydrophobic stripe between two hydrophilic stripes is studied both experimentally and numerically. The capillary bridge is formed from an evaporating water droplet wetting three neighboring stripes of a chemically patterned surface. The simulations are based on the Volume-of-Fluid (VOF) method implemented in Free Surface 3D (FS3D). By considering the breakup process in phase space, the breakup dynamics can be evaluated without the uncertainty in determining the precise breakup time. It is found that within an intermediate inviscid regime, the breakup dynamics follows a  $t^{2/3}$ -scaling, indicating that the breakup process is dominated

by the balance of inertial and capillary forces. For smaller bridge widths, the breakup velocity reaches a plateau, which is due to viscous forces becoming more important. In the final stage of breakup, the capillary bridge forms a liquid thread that breaks up consistent with the Rayleigh-Plateau instability. The existence of satellite droplets in a regular pattern indicates that the primary breakup process is followed by self-similar secondary breakups.

CPP 3.2 Mon 9:20 CPPb

**Simulating the hydrodynamics of droplets on photo-switchable substrates** — ●JOSUA GRAWITTER and HOLGER STARK — Technische Universität Berlin, Institute of Theoretical Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Interfaces between fluids and photo-switchable substrates provide a unique mechanism to precisely manipulate liquid droplets by creating and adapting a heterogeneous wettability landscape. Because droplets respond to changes in wettability, such interfaces provide a means to keep the droplets in non-equilibrium and thereby induce new states of

dynamic wetting.

We present a boundary element method to determine the Stokes flow inside a droplet with its curved free surface and its flat interface at the substrate, where we apply the Navier boundary condition to permit motion of the contact line. In our approach we use the Cox-Voinov law [1] and introduce the velocity of the contact-line as a side condition. We also implement an iterative domain-splitting integration scheme capable of treating singular integrands, which are typical for the boundary element method. Using the implemented method, we study how droplets respond to specific spatiotemporal wettability patterns that either move or deform the droplet. Here, we present first studies of the spatio-temporal deformation dynamics induced by oscillating wettability along the contact line and of directed motion initiated by traveling wettability patterns. We specifically investigate how to design the patterns in order to maximize droplet speed.

[1] O. V. Voinov, *Fluid Dyn.* **11**, 714 (1976).

CPP 3.3 Mon 9:40 CPPb

**Dynamics of liquid droplets on switchable prestructured substrates** — ●MORITZ STIENEKER<sup>1</sup> and SVETLANA GUREVICH<sup>1,2</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, D-48149 Münster, Germany — <sup>2</sup>Center for Nonlinear Science (CeNoS), University of Münster, Corrensstrasse 2, D-48149 Münster, Germany

A mesoscopic continuum model is employed to model a thin, liquid film on a substrate with a spatio-temporal wettability. In particular, the effect of a switchable wettability pattern on the structure formation is analyzed for a one-dimensional case with the help of path-continuation techniques and direct numerical time simulations. It is found that if the periodic switching is introduced, the system reaction depends on the ratio between the time scale given by switching and the reaction time of the liquid. The behaviour of the contact angle during the slow and fast switching is investigated in details. Furthermore it is demonstrated that in the case of the slow switching the droplet solutions corresponding to the local minima of the free energy can be stabilized.

CPP 3.4 Mon 10:00 CPPb

**Gradient dynamics model for drops spreading on polymer brushes** — ●SIMON HARTMANN and UWE THIELE — Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Deutschland

When a liquid drop spreads on an adaptive substrate the latter changes its properties what may result in an intricate coupled dynamics of drop and substrate. We present a generic mesoscale hydrodynamic model for such processes that is written as a gradient dynamics on an underlying energy functional. We specify the model details for the example of a drop spreading on a dry polymer brush. There, liquid absorption into the brush results in swelling of the brush causing changes in the brush topography and wettability. The liquid may also advance within the brush via diffusion (or wicking) resulting in coupled drop and brush dynamics. The specific model accounts for coupled spreading, absorption and wicking dynamics when the underlying energy functional incorporates capillarity, wettability and brush energy. We employ a simple version of such a model to numerically simulate a droplet spreading on a swelling brush and provide an in-depth analysis of the simulation results and some interesting quantities.

40 min. meet the speakers - break

Invited Talk

CPP 3.5 Mon 11:00 CPPb

**Liquid-liquid Dewetting: From Spinodal Breakup to Dewetting Morphologies and Rates** — ●RALF SEEMANN<sup>1</sup>, ROGHAYEH SHIRI<sup>1</sup>, STEFAN BOMMER<sup>1</sup>, DIRK PESCHKA<sup>2</sup>, SEBASTIAN JACHALSKI<sup>2</sup>, LENOIE SCHMELLER<sup>2</sup>, and BARBARA WAGNER<sup>2</sup> — <sup>1</sup>Saarland University, Experimental Physics, D-66123 Saarbrücken — <sup>2</sup>Weierstrass Institute, Mohrenstr. 39, D-10117 Berlin

The dewetting of liquid polystyrene (PS) from liquid polymethylmethacrylate (PMMA) is studied. At dewetting temperatures, both polymers can be considered as Newtonian fluids with the same viscosity. Provided that the liquid PS layer is below 10 nm, breakup occurs by spinodal dewetting. Due to the low interfacial tension of the buried interface compared to the PS-air interface and the large mobility, a very short spinodal wavelength develops with a larger amplitude of the buried interface than that of the free PS-air interface. The spinodal patterns of PMMA-PS and PS-air interface are anti-correlated and the observed wavelength is within the range predicted from thin

film models. For a later dewetting stage, when dewetting rims in the range of the PMMA film thickness have formed, characteristic profiles of both PMMA-PS and PS-air interface develop, which depend on the PMMA/PS thickness ratio. The dewetting rates are approximately linear but do not obey any well-defined scaling behavior. Based on the agreement of experimental results with theoretical predictions, we use the numerical simulations to predict local flow fields and energy dissipation that would otherwise be inaccessible to experiments.

CPP 3.6 Mon 11:40 CPPb

**Wetting transitions on soft substrates** — MAREK NAPIORKOWSKI<sup>1</sup>, ●LOTHAR SCHIMMELE<sup>2</sup>, and SIEGFRIED DIETRICH<sup>2,3</sup> — <sup>1</sup>Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland — <sup>2</sup>Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — <sup>3</sup>IV. Institut für Theoretische Physik, Universität Stuttgart, Stuttgart, Germany

Within mean-field theory we study wetting of elastic substrates. Our analysis is based on a grand canonical free energy functional of the fluid number density and of the substrate displacement field. The substrate is described in terms of the linear theory of elasticity, parametrized by two Lamé coefficients. The fluid contribution is of the van der Waals type. Two potentials characterize the interparticle interactions in the system, the long-ranged attraction between the fluid particles and a potential characterizing the substrate-fluid interaction. By integrating out the elastic degrees of freedom we obtain an effective theory for the fluid number density alone. Its structure is similar to the one for wetting of an inert substrate. However, the long-ranged attraction between the fluid particles is replaced by an effective potential which also contains a term bilinear in the substrate-fluid interaction.

We discuss the corresponding wetting transitions in terms of an effective interface potential depending on the thickness of the wetting layer. We show that in the case of algebraically decaying interactions the elasticity of the substrate may suppress critical wetting transitions, and may even turn them first order.

CPP 3.7 Mon 12:00 CPPb

**A Thermodynamic Consistent, Instantaneous Dividing Surface to Study Wetting Phenomena** — ●AMAL KANTA GIRI and MARCELLO SEGA — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

A detailed knowledge of the microscopic structure and dynamics in the interfacial region of soft materials is a necessary step on the way to develop novel materials and is also key to a deeper understanding of the statistical mechanics of fluid interfaces out of equilibrium. The presence of thermal capillary waves, however, hinders efforts to investigate the local structure of interfaces by smearing out observable quantities computed in the global reference frame. To recover a detailed picture of the interface neighborhood, one needs to compute observables in the local, instantaneous reference frame located at the interface, although the determination of this frame is, in general, not unique.

Here, we report on the possibility of using computational geometry approaches to determine the set of instantaneous surface atoms in a way which is thermodynamically consistent with the Gibbs (equimolar) dividing surface. We apply these methods to the determination of the instantaneous, fluctuating contact line of droplets on solid substrates, with an outlook on the problem of dynamic wetting of soft, deformable substrates.

CPP 3.8 Mon 12:20 CPPb

**Core-shell latex colloids as interfaces for tailoring wetting properties** — CALVIN J. BRETT<sup>1,2,3</sup>, JOAKIM ENGSTRÖM<sup>3,4</sup>, VOLKER KÖRSTGENS<sup>5</sup>, PETER MÜLLER-BUSCHBAUM<sup>5,6</sup>, EVA MALMSTRÖM<sup>4</sup>, and ●STEPHAN V. ROTH<sup>1,4</sup> — <sup>1</sup>DESY, 22603 Hamburg, Germany — <sup>2</sup>KTH, Dept. Mechanics, SE-10044 Stockholm, Sweden — <sup>3</sup>WWSC, SE-10044 Stockholm, Sweden — <sup>4</sup>KTH, Dept. Fibre and Polymer Technology, SE-10044 Stockholm, Sweden — <sup>5</sup>TUM, Physik Department, 85748 Garching, Germany — <sup>6</sup>MLZ, TUM, 85748 Garching, Germany

Facile surface functionalisation of latex colloids makes them most promising materials for broad thin film applications. However, the effect of these colloids on chemical film and wetting properties is not easily evaluated. Core-shell particles can deform and coalesce on the nanoscale during thermal annealing yielding tailored physical properties. We investigated two different core-shell systems (soft and rigid) with identical shell but with chemically different core polymer and core size. These core-shell colloids are probed during thermal anneal-

ing on surfaces in order to investigate their behavior as a function of nanostructure size and rigidity. X-ray scattering allows us to follow the re-arrangement of the colloids and the structural evolution in situ during annealing. Evaluation by real-space imaging techniques reveals a disappearance of the structural integrity and a loss of colloids' boundaries. We present the possibility to tailor and fine-tune the wettability by tuning the core-shell colloid morphology in thin films, thus providing a facile template methodology for repellent surfaces.

CPP 3.9 Mon 12:40 CPPb

**Drop Impact on Hot Plates: Contact, Lift-Off and the Formation of Holes** — ●KIRSTEN HARTH<sup>1,2</sup>, SANG.HYEON LEE<sup>3</sup>, MAAIKE RUMP<sup>2</sup>, MINWOO KIM<sup>3</sup>, DETLEF LOHSE<sup>2</sup>, KAMEL FEZZAA<sup>4</sup>, and JUNG HO JE<sup>3</sup> — <sup>1</sup>Institute of Physics, Otto von Guericke University Magdeburg — <sup>2</sup>Physics of Fluid and Max Planck Center, University of Twente, The Netherlands — <sup>3</sup>X-Ray Imaging Center, Pohang University of Science and Technology, Korea — <sup>4</sup>X-Ray Science Division, Argonne Ntnl. Laboratory, USA

Everyone who poured water into a hot pan has experienced the manifold boiling behaviours of drops impacting on a hot plate, a problem which is of high relevance in many technical applications. When the drop is gently deposited, and the surface temperature is sufficiently high, it hovers on a vapour layer (Leidenfrost effect). For impacting drops, this critical temperature for a contact-less rebound is substantially increased, and much harder to determine. In fact, determining contact times between drops and smooth substrates from side view imaging is impossible for most temperatures above the boiling point.

We combine High-Speed Total Internal Reflection and synchrotron X-Ray measurements to reliably determine contact times and the Leidenfrost temperature for drops impacting on smooth hot surfaces. Furthermore, we study the lift-off characteristics. A local minimum in lift-off times correlates with spontaneous lamella rupture and the morphology of the contact.

60 min. meet the speakers - break

Invited Talk

CPP 3.10 Mon 14:00 CPPb

**Sinking droplet durotaxis and engulfment** — ●ANNE JUEL — Department of Physics & Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Durotaxis refers to the spontaneous motion of objects along stiffness gradients of the supporting substrate. In droplet durotaxis migration occurs down rigidity gradients towards the softer regions of the substrate due to elasto-capillary interaction. We perform experiments in the limit of very soft PDMS substrates, where the cross-linked matrix of the gel can yield under the capillary stresses exerted by the sessile droplet. We find that the droplet moves towards the softest i.e. deepest parts of the gel layer while also sinking into the gel and that droplet durotaxis is much faster when engulfment is associated with the motion. For comparison, we focus on engulfment of aqueous droplets deposited onto a substrate layer of silicone oil. On substrates with a depth gradient, we observe qualitatively similar behaviour to the sinking durotaxis case. On deep layers, the droplet is ultimately engulfed in the oil layer. This involves rapid submersion of the droplet driven by capillary forces in the oil surface, followed by the much slower peeling of the droplet from the interface to which it is adhered. The later peeling stage is driven by a combination of geometric constraints at the apparent contact line and gravity pulling on the droplet. Gravitational effects are therefore essential to complete engulfment, even for micrometric droplets. Furthermore, the opposing effects of geometry and gravity result in the longest engulfment times for droplets of intermediate size.

CPP 3.11 Mon 14:40 CPPb

**Droplets fighting contamination** — ●ABHINAV NAGA, WILLIAM WONG, ANKE KALTBEITZEL, MARIA D'ACUNZI, HANS-JÜRGEN BUTT, and DORIS VOLLMER — Max Planck Institute for Polymer Research, Mainz, Germany

Lubricated surfaces are prone to accumulating contaminants due to their sticky yet slippery nature. The presence of contaminants, such as dust and dirt particles, alters their performance. An understanding of the effect of contaminated particles on the friction of surfaces is important not only from a fundamental perspective whereby further insight can be gained of the underlying mechanisms, but also from an applied perspective to predict the effectiveness of lubricated surfaces in the presence of contaminants.

In this study, we systematically contaminate lubricated silicone surfaces (Sylgard 184) and non-lubricated surfaces with spherical glass microparticles. We place a droplet on each surface and measure the force needed to push the droplet at different speeds towards an individual microparticle. We visualise this process with laser scanning confocal microscopy, focusing on the deformation inflicted by the microparticle on the droplet and its lubricant ridge. We combine these visualisations with our force measurements to suggest a mechanism for the removal of contaminated particles from surfaces using droplets, and we outline the differences between the outcomes on the lubricated and the non-lubricated surfaces. This work will help to understand droplet dynamics on imperfect or dirty lubricated surfaces.

CPP 3.12 Mon 15:00 CPPb

**Lucas-Washburn equation applies for four phase contact point** — ●PEYMAN ROSTAMI<sup>1,2</sup> and GÜNTER AUERNHAMMER<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, 55128, Mainz, Germany — <sup>2</sup>Leibniz Institute of Polymer Research, 01069, Dresden, Germany

A four-phase contact point, e.g., in merging of immiscible drops, is the point where the liquid-liquid interface advances along the contact line of one drop. The dynamics of drop merging involve various driving and dissipating forces in the dynamics of the four-phase contact point. The viscous friction, i.e. the flow field, within liquids is influenced by the different boundary conditions on the different interfaces (liquid-gas, liquid-liquid, liquid-solid). Additionally, Marangoni stresses between the two liquids and the spreading coefficients along the contact lines play a role. Effectively, these effects lead to a capillary force acting on the four-phase contact point. In total, the situation resembles the capillary flow in open V-shaped groove. The important difference is that, in the classical problem, the grooves are made out of two solid walls, but in the present case one of the \*walls\* is liquid, i.e., flowable and deformable. We investigate a range of liquids with different combination of physical properties (viscosity ratio, surface and interfacial tensions). The results show a good qualitative agreement for different liquids of the experimental results with the classical Washburn equation ( $h \sim \sqrt{\text{time}}$ ), where  $h$  is the filled length of the \*groove\*.

CPP 3.13 Mon 15:20 CPPb

**Imbibition-Induced Deformation Dynamics in Nanoporous Media** — ●JUAN SANCHEZ<sup>1</sup>, ZHUOQING LI<sup>2</sup>, MICHAEL FROEBA<sup>3</sup>, and PATRICK HUBER<sup>4</sup> — <sup>1</sup>Institute of Materials Physics, Hamburg University of Technology — <sup>2</sup>Institute of Materials Physics, Hamburg University of Technology — <sup>3</sup>Institute of Anorganic and Applied Chemistry, Hamburg University — <sup>4</sup>Institute of Materials Physics, Hamburg University of Technology

We present time-dependent macroscopic dilatometry experiments on the deformation of nanoporous monoliths (carbon and silica) upon spontaneous, capillarity-driven invasion of water. We find two distinct dynamical regimes. One of them can be quantitatively traced to deformations originating in changes in the surface stress at the inner pore walls (dynamic Bangham's regime) upon water invasion, whereas the second one results from Laplace pressure effects. Our study demonstrates that it is possible to dynamically monitor imbibition dynamics by simple dilatometry measurements.

CPP 3.14 Mon 15:40 CPPb

**Macroscopic Capillary Number for Characterization of Two-phase Flow in Porous Media** — ●HU GUO and RUDOLF HILFER — Institute for Computational Physics, Universität Stuttgart, Stuttgart, Germany

The Capillary number ( $Ca$ ) defined as the ratio of viscous force to capillary force is widely used to qualitatively characterize multiphase flow in porous media as in carbon dioxide geologic sequestration and chemical enhanced oil recovery (EOR). The main difficulty is to characterize forces properly. There exists 22 definitions for  $Ca$  (Guo et al, IOR 2020). The most concise definition is  $Ca = \frac{v\mu}{\sigma}$  with velocity  $v$ , viscosity  $\mu$  and interfacial tension  $\sigma$  (Saffman and Taylor, 1958). It is supported by core flooding tests and most widely used. However, this definition is less sound than the one that involves the wettability parameter (Moore and Slobod, 1955). Meanwhile, the values of these  $Ca$  are regarded as too small to reflect the actual force balance (Dullien, 1979). It was shown theoretically, that this  $Ca$  is microscopic in nature and incorrectly used (Hilfer and Øren, 1996, Trans. Porous Media).

We study the new macroscopic capillary number  $Ca = \frac{\mu\phi v L}{K P_b}$  with viscosity  $\mu$ , porosity  $\phi$ , velocity  $v$ , permeability  $K$ , length  $L$  and capil-

lary breakthrough pressure  $P_b$  (Hilfer et al, 2015, Physical Review E). The new  $Ca$  explains some of the latest observations (Doorwar and Mohanty, 2017, SPE J; Qi et al, 2017, SPE J; Rabbani et al, 2018, PNAS; Zhao et al, 2019, PNAS) that contradict predictions obtained

from the microscopic  $Ca$ . EOR field practice also verified that the macroscopic  $Ca$  is more profound.

**30 min. meet the speakers - break**

## CPP 4: Active Biological Matter I (joint session BP/DY/ CPP)

Time: Monday 9:00–11:00

Location: BPb

### Invited Talk

CPP 4.1 Mon 9:00 BPb

**The tortoise and hare: how moving slower allows groups of bacteria to spread across surfaces** — OLIVER MEACOCK<sup>1,2</sup>, AMIN DOOSTMOHAMMADI<sup>3</sup>, KEVIN FOSTER<sup>1</sup>, JULIA YEOMANS<sup>1</sup>, and WILLIAM DURHAM<sup>1,2</sup> — <sup>1</sup>University of Oxford, United Kingdom — <sup>2</sup>University of Sheffield, United Kingdom — <sup>3</sup>University of Copenhagen, Denmark

Bacteria use tiny grappling hook like appendages called pili to pull themselves across solid surfaces. While pili-based motility has been widely studied in solitary *Pseudomonas aeruginosa* cells, this species also uses pili to collectively migrate across surfaces when they are densely packed together in a colony. Interestingly, we find genotypes that individually move slower can collectively migrate faster as a group. Using theory developed to study liquid crystals, we demonstrate that this effect is mediated by the physics of topological defects, points where cells with different orientations meet one another. Our analyses reveal that when defects with a topological charge of  $+1/2$  collide with one another, the fast-moving mutant cells rotate vertically and become trapped. By moving more slowly, wild-type cells avoid this trapping mechanism, allowing them to collectively migrate faster. Our work suggests that the physics of liquid crystals has played a pivotal role in the evolution of collective bacterial motility by exerting a strong selection for cells that exercise restraint in their movement.

Full paper in Nature Physics available free of charge at: <https://rdcu.be/cbcgc>

CPP 4.2 Mon 9:30 BPb

**Light-regulated cell aggregation in confinement** — ALEXANDROS FRAGKOPOULOS<sup>1</sup>, JEREMY VACHIER<sup>1</sup>, JOHANNES FREY<sup>1</sup>, FLORA-MAUD LE MENN<sup>1</sup>, MARCO MAZZA<sup>1,2</sup>, MICHAEL WILCZEK<sup>1</sup>, DAVID ZWICKER<sup>1</sup>, and OLIVER BÄUMCHEN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Dynamics and Self-Organization (MPIDS), D-37077 Göttingen, Germany — <sup>2</sup>Department of Mathematical Sciences, Loughborough University, Loughborough, Leicestershire LE11 3TU, United Kingdom — <sup>3</sup>Experimental Physics V, University of Bayreuth, D-95447 Bayreuth, Germany

Photoactive microbes live in complex environments with spatially and temporally fluctuating light conditions. They survive in such habitats by switching their metabolic activity from photosynthesis to aerobic respiration in unfavorable light conditions. We demonstrate that this adaptation in a suspension of soil-dwelling *Chlamydomonas reinhardtii* cells under confinement leads to a spontaneous separation into regions of high and low cell densities. We show that the inhibition of the photosynthetic machinery is necessary but insufficient to generate the observed aggregation. Microfluidic experiments, simulations, and mean-field theory approaches demonstrate that the emergence of microbial aggregations is governed by the oxygen concentration field inside the microhabitat. In fact, in regions where the energy production is completely arrested by both, the photosynthetic and respiratory systems, the cell speed decreases resulting in an aggregation, which thus takes

the form of the underline oxygen field.

CPP 4.3 Mon 9:50 BPb

**Emergent activity of motile phytoplankton in nutrient landscapes** — JAYABRATA DHAR, FRANCESCO DANZA, ARKAJYOTI GHOSHAL, and ANUPAM SENGUPTA — Physics of Living Matter Group, Department of Physics and Materials Science, University of Luxembourg, 162 A, Avenue de la Faencerie, L-1511, Luxembourg City, Luxembourg

Despite their minuscule size, microbes mediate a range of processes in ecology, medicine, and industrial settings that span orders of nutrient concentrations. Yet, to date, we lack a biophysical framework that could link nutrient availability to phytoplankton behavior and predict the impact of dynamic nutrient conditions on motility. Using a combination of micro-scale imaging, microbiology and fluid dynamic models, we quantify how nutrient availability regulates motility, at both individual and population scales [1]. We extract the time-scales over which phytoplankton actively regulate swimming and morphological characteristics, thus shedding light on the finely tuned biophysical mechanisms that equip cells to tackle spatial and temporal heterogeneity of nutrient landscapes. Our results propose local nutrient levels as a handle to control the activity of motile phytoplankton species, promising an exciting model of tunable motile active matter.

[1] Danza, Dhar, Ghoshal and Sengupta (in prep.)

CPP 4.4 Mon 10:10 BPb

**Chemotaxis strategies of bacteria with multiple run-modes** — ZAHRA ALIREZAEIZANJANI<sup>1,2</sup>, ROBERT GROSSMANN<sup>1</sup>, VERONIKA PFEIFER<sup>1</sup>, MARIUS HINTSCHE<sup>1</sup>, and CARSTEN BETA<sup>1</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — <sup>2</sup>Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany

Bacterial chemotaxis – a fundamental example of directional navigation in the living world – is key to many biological processes, including the spreading of bacterial infections. Many bacterial species were recently reported to exhibit several distinct swimming modes – the flagella may, for example, push the cell body or wrap around it. How do the different run modes shape the chemotaxis strategy of a multi-mode swimmer? Here, we investigate chemotactic motion of the soil bacterium *Pseudomonas putida* as a model organism. By simultaneously tracking the position of the cell body and the configuration of its flagella, we demonstrate that individual run modes show different chemotactic responses in nutrition gradients and thus constitute distinct behavioral states. Based on an active particle model, we demonstrate that switching between multiple run states that differ in their speed and responsiveness provide the basis for robust and efficient chemotaxis in complex natural habitats.

**30 min. Meet the Speaker**

## CPP 5: Active Biological Matter II (joint session BP/ CPP/DY)

Time: Monday 11:00–13:30

Location: BPb

CPP 5.1 Mon 11:00 BPb

**Chiral stresses in nematic cell monolayers** — LUDWIG A. HOFFMANN<sup>1</sup>, KOEN SCHAKENRAAD<sup>1,2</sup>, ROELAND M. H. MERKS<sup>2,3</sup>, and LUCA GIOMI<sup>1</sup> — <sup>1</sup>Instituut-Lorentz, Leiden University, The Netherlands — <sup>2</sup>Mathematical Institute, Leiden University, The Netherlands — <sup>3</sup>Institute of Biology, Leiden University, The Netherlands

Recent experiments on monolayers of spindle-like cells have provided

a convincing demonstration that certain types of collective phenomena in epithelia are well described by active nematic hydrodynamics. While recovering some of the predictions of this framework, however, these experiments have also revealed unexpected features that could be ascribed to the existence of chirality over length scales larger than the typical size of a cell.

We elaborate on the microscopic origin of chiral stresses in nematic cell monolayers and investigate how chirality affects the motion of



topological defects, as well as the collective motion in stripe-shaped domains. We find that chirality introduces a characteristic asymmetry in the collective cellular flow, from which the ratio between chiral and non-chiral active stresses can be measured. Furthermore, we find that chirality changes the nature of the spontaneous flow transition under confinement and that, for specific anchoring conditions, the latter has the structure of an imperfect pitchfork bifurcation.

CPP 5.2 Mon 11:20 BPb

**Developmentally driven self-assembly of living chiral crystals** — ●ALEXANDER MIETKE<sup>1</sup>, TZER HAN TAN<sup>2</sup>, HUGH HIGINBOTHAM<sup>2</sup>, YUCHAO CHEN<sup>2</sup>, PETER FOSTER<sup>2</sup>, SHREYAS GOKHALE<sup>2</sup>, JÖRN DUNKEL<sup>1</sup>, and NIKTA FAKHRI<sup>2</sup> — <sup>1</sup>Department of Mathematics, Massachusetts Institute of Technology, Cambridge, MA — <sup>2</sup>Department of Physics, Massachusetts Institute of Technology, Cambridge, MA

The emergent dynamics exhibited by self-organizing collections of living organisms often shows signatures of symmetries that are broken at the single-organism level. At the same time, early organism development itself is accompanied by a sequence of symmetry breaking events that eventually establish the body plan. Combining these key aspects of collective phenomena and embryonic development, we describe here the spontaneous formation of hydrodynamically stabilized active crystals made of hundreds of starfish embryos during early development. As development progresses and embryos change morphology, crystals become increasingly disordered and eventually stop forming. We show that these structures exhibit distinct macroscopic chiral features as a direct consequence of the embryo's chiral swimming properties. We introduce a hydrodynamic near-field model that quantitatively describes the formation and rotation of crystals, as well as the emergence of long-lived chiral deformation waves, all of which can be understood as consequences of broken symmetries on the single-embryo level.

CPP 5.3 Mon 11:40 BPb

**Thin-Film Model of Resting and Moving Active Droplets** — ●FENNA STEGEMERTEN<sup>1</sup>, SARAH TRINSHECK<sup>1,2</sup>, KARIN JOHN<sup>2</sup>, and UWE THIELE<sup>1,3</sup> — <sup>1</sup>Institut für Theoretische Physik, Westfälische Wilhelms-Universität Münster, Münster, Germany — <sup>2</sup>Université Grenoble-Alpes, CNRS Laboratoire Interdisciplinaire de Physique, Grenoble, France — <sup>3</sup>Center for Nonlinear Science (CeNoS), Westfälische Wilhelms-Universität Münster, Münster, Germany

We propose a long-wave model for free-surface drops of polar active liquid on a solid substrate. The coupled evolution equations for the film height and the local polarization profile are written in the form of a gradient dynamics supplemented with active stresses and fluxes. A wetting energy for a partially wetting liquid is incorporated allowing for motion of the liquid-solid-gas contact line. This gives a consistent basis for the description of drops of dense bacterial suspensions or compact aggregates of living cells on solid substrates. As example, we analyze the dynamics of active drops and demonstrate how active forces compete with passive surface forces to shape droplets and drive contact line motion. We perform parameter continuation in the activity parameters discussing both, resting and moving droplets. Additional direct time simulations investigate transitions from non-uniformly to uniformly polarized as well as resting to moving states.

CPP 5.4 Mon 12:00 BPb

**Sedimentation and Convection of Bottom-Heavy Squirmer** — ●FELIX RÜHLE, JAN-TIMM KUHR, and HOLGER STARK — TU Berlin, Institut für Theoretische Physik, Berlin, Germany

Active particles form appealing patterns, in particular, when hydrodynamic interactions are present [1-3]. A fascinating example known from biology is bioconvection of microswimmers under gravity [4]. In order to study such systems, we simulate bottom-heavy squirmers (neutral squirmers, pushers, and pullers) under different gravitational forces and torques [3]. The relevant parameters are the ratio of swimming to bulk sedimentation velocity  $\alpha$  and the normalized torque.

In the state diagram of these parameters, for neutral squirmers at

low  $\alpha$  we observe sedimentation states, where bottom-heaviness leads to the formation of clusters of different sizes. For high  $\alpha$ , finite torques lead to inverted sedimentation. In between, we identify plumes of collectively sinking squirmers that feed convective rolls of circling squirmers at the bottom of the simulation cell. At  $\alpha \gtrsim 1$  and large torques squirmers form a spawning cluster above the wall, from which squirmers occasionally escape. For strong pushers and pullers, we find that the dipolar flow fields weaken the formation of plumes and convective rolls.

[1] M. Hennes, *et al.*, PRL **112**, 238104 (2014)

[2] H. Jeckel, *et al.*, PNAS **116**, 1489 (2019).

[3] F. Rühle, and H. Stark, Eur. Phys. J. E **43**, 26 (2020).

[4] T.J. Pedley, and J.O. Kessler, Annu. Rev. Fluid Mech. **24**, 313 (1992).

CPP 5.5 Mon 12:20 BPb

**Microscopic scattering of pusher particles in complex environments** — ●THERESA JAKUSZEIT<sup>1</sup>, SAMUEL BELL<sup>2</sup>, and OTTAVIO A. CROZE<sup>1</sup> — <sup>1</sup>Cavendish Laboratory, JJ Thomson Avenue, CB3 0HE, Cambridge, United Kingdom — <sup>2</sup>Laboratoire Physico Chimie Curie, Institut Curie, PSL Research University, CNRS UMR168, 75005 Paris, France

Active propulsion as performed by bacteria and Janus particles, in combination with hydrodynamic interaction at boundaries, can lead to the breaking of time reversibility. One typical example of this is the accumulation of bacteria on a flat wall. However, in microfluidic devices with cylindrical pillars of sufficiently small radius, self-propelled particles can slide along the surface of a pillar without becoming trapped over long times. This non-equilibrium scattering process can result in large diffusivities even at high obstacle density, unlike particles that undergo classical specular reflection, as in the Lorentz gas. We experimentally study the non-equilibrium scattering as well as the long-term diffusive transport of pusher-like particles by tracking wild-type and smooth-swimming mutants of the model bacterium *Escherichia coli* in microfluidic obstacle lattices. We relate the determined parameters of the scattering process to previously proposed models and discuss their relevance. Finally, we discuss the potential interpretation of the role of tumbles in the scattering process.

CPP 5.6 Mon 12:40 BPb

**Swimming behavior of squirmer dumbbells and polymers** — ●JUDIT CLOPÉS LLAHÍ, GERHARD GOMPPER, and ROLAND G. WINKLER — Theoretical Soft Matter and Biophysics, Institute for Advanced Simulation and Institute of Complex Systems, Forschungszentrum Jülich, D-52425 Jülich, Germany

Nature provides a plethora of microswimmers, which can be rather elongated, filament- or polymer-like. Examples are bacteria swarmer cells or marine phytoplankton dinoflagellates assembling in a linear fashion. In order to address the relevance of hydrodynamic interactions for the collective behavior of such organisms, we study the swimming properties of linear polymer-like assemblies by mesoscale hydrodynamic simulations, where an active unit (monomer) is described by a spherical squirmer – which can be a pusher, a neutral swimmer, or a puller. We find that the monomer hydrodynamic flow field leads to correlations in the relative orientation of adjacent monomers, and consequently the swimming efficiency differs from that of active Brownian linear assemblies. In particular, puller dumbbells and chains show a pronounced increase in the rotational diffusion coefficient compared to pushers, while for neutral squirmers, the rotational diffusion coefficient is similar to that of active Brownian particles. Hence, the large-scale conformational and dynamical properties depend on the specific propulsion mechanism. Refs.: J. Elgeti, R. G. Winkler, G. Gompper, Rep. Prog. Phys. **78**, (2015). R. G. Winkler, J. Elgeti, G. Gompper, J. Phys. Soc. Jpn. **86**, (2017). J. Clopés, G. Gompper, R. G. Winkler, Soft Matter **16**, 10676 (2020).

**30 min. Meet the Speaker**

## CPP 6: Poster Session I - Molecular Electronics and Wetting

Time: Monday 16:30–18:30

Location: CPPp

CPP 6.1 Mon 16:30 CPPp

**Azobenzene molecular switches: Testing the charge transport in a self-assembled monolayer under light stimulus** — ●VLADYSLAV SAVCHENKO and OLGA GUSKOVA — Leibniz Institute of Polymer Research Dresden (IPF Dresden), Hohe Str. 6, Dresden

The azobenzene-based molecules organized in chemisorbed self-assembled monolayers (SAMs) on the surfaces of electrodes work as photoswitches of the conductance, the electrode work function, and the magnetization/magnetic transitions. The aim of this computational study is to predict how the configurational rearrangements of the building blocks in a molecular switch consisting of azobenzene moiety and bithiophene spacer linked to a short alkanethiol affect the structural, electronic, and transport properties in SAMs.

The financial support of the Deutsche Forschungsgemeinschaft, project GU1510 5-1 "Optically reconfigurable nanoscale junctions for organic electronics" is highly appreciated.

CPP 6.2 Mon 16:30 CPPp

**Ordered donor-acceptor complex formation and electron transfer in co-deposited films of structurally dissimilar molecules** — ●ANDREAS OPITZ<sup>1</sup>, C. PETER<sup>1</sup>, B. WEGNER<sup>1,2</sup>, H.S.S.R. MATTE<sup>1</sup>, A. RÖTTGER<sup>1</sup>, T. FLORIAN<sup>1</sup>, X. XU<sup>1</sup>, P. BEYER<sup>1</sup>, L. GRUBERT<sup>1</sup>, S. HECHT<sup>1</sup>, V. BELOVA<sup>3</sup>, A. HINDERHOFER<sup>3</sup>, F. SCHREIBER<sup>3</sup>, C. KAPSER<sup>4</sup>, J. PFLAUM<sup>4</sup>, Y. ZHANG<sup>5</sup>, S. BARLOW<sup>5</sup>, S.R. MARDER<sup>5</sup>, and N. KOCH<sup>1,2</sup> — <sup>1</sup>Humboldt-Universität zu Berlin — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie — <sup>3</sup>Universität Tübingen — <sup>4</sup>Universität Würzburg — <sup>5</sup>Georgia Institute of Technology Atlanta (USA)

Electrical and optoelectronic properties of organic semiconductor thin films can be tailored by co-deposition of molecular materials. At the moment it is difficult to predict a priori the resulting morphology (like phase separation or mixed crystals) for a selected material combination. Here, we study electron transfer between planar, rod-like electron donor molecules (DIP, PEN, DBTTF) and a non-planar electron acceptor molecule [Mo(tfd)<sub>3</sub>] in co-evaporated films by analyzing morphological, vibrational and optical properties. [1]

The resulting morphology of the co-deposited films (phase separation or mixed crystals) can be rationalized within the laws of thermodynamics. Therefore, it is necessary to consider structural incompatibility of the molecules in terms of interaction energies between the molecules as well as the Coulomb attraction between molecular ions after the formation via ground-state electron transfer.

[1] A. Opitz et al., *J. Phys. Chem. C* **124** (2020) 11023-11031.

CPP 6.3 Mon 16:30 CPPp

**Solid-state effects in the electronic and optical properties of donor-acceptor co-crystals** — ●MICHELE GUERRINI<sup>1,2</sup>, ANA M. VALENCIA<sup>1,2</sup>, and CATERINA COCCHI<sup>1,2</sup> — <sup>1</sup>Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany — <sup>2</sup>Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

In the framework of density functional theory and many-body perturbation theory, we investigate the role of solid-state effects (SSEs) in the electronic and optical properties of a donor-acceptor (DA) co-crystal composed of quarterthiophene donor molecules p-doped by (fluorinated)-tetracyanoquinodimethane. We find that the hybridization of the frontier electronic states is hindered along specific directions in the crystal cell, in favor of segregated states. We rationalize this behavior in terms of wave-function delocalization in the co-crystals competing and prevailing over the local interactions at the DA interfaces [1,2].

The anisotropic optical absorption spectra of the co-crystals are highly anisotropic and are dominated by a bright charge-transfer exciton at lowest-energy polarized along the direction of the DA stacks.

Our result contribute to rationalize the fundamental mechanisms ruling the formation of charge-transfer excitons in DA co-crystals.

[1] A M Valencia and C Cocchi, *JPC* 2019, 123, 9617

[2] A M Valencia; M Guerrini and C Cocchi, *PCCP* 2020, 22, 3527

CPP 6.4 Mon 16:30 CPPp

**Uncovering the enhancement mechanisms of thermoelectric performance of PEDOT: PSS films after physical-chemical**

**dedoping** — SUO TU, TING TIAN, ANNA-LENA OECHSLE, and ●PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany

PEDOT: PSS is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility in thermoelectric (TE) devices. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT and defined as  $ZT = S^2\sigma T/k$  where S is the Seebeck coefficient,  $\sigma$  is the electrical conductivity, T is the absolute temperature, k is the thermal conductivity, and  $S^2\sigma$  is defined as the power factor (PF). Nevertheless, it is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the parameters S,  $\sigma$ , and k are interdependence as a function of carrier concentration and hard to be optimized simultaneously. In this work, we adopt a combination of DMSO addition and subsequent DMSO/salt mixture post-treatment to engineer TE performance of PEDOT: PSS thin films. Results show that the as-obtained PEDOT: PSS film presents a maximum PF of 105.2  $\mu\text{W}/(\text{m}\cdot\text{K}^2)$ , which is  $\sim 1750$ -fold larger than that of pristine film. The origin and mechanism of the underlying improvement is systematically investigated by various characterizations to gain a more profound understanding of the fundamental nature of modified PEDOT: PSS films.

CPP 6.5 Mon 16:30 CPPp

**Dependence of Electron and Ion Transport on the Intermolecular Coupling in Fluorinated Phthalocyanine Thin Films as Electrochromic Materials** — ●THI HAI QUYEN NGUYEN<sup>1</sup>, MARIUS PELMUS<sup>2</sup>, MICHAEL SCHÄFER<sup>1</sup>, SERGIU M. GORUN<sup>2</sup> und DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Justus Liebig University Giessen, Institute of Applied Physics — <sup>2</sup>Seton Hall University, Department of Chemistry and Biochemistry

Phthalocyanines as organic ionic and electronic conductors are of great interest for the application in electrochromic devices. An influence of the degree of fluorination in copper phthalocyanines on the intermolecular coupling in the solid state and, thus, on the rate of electron and ion transport was observed: For  $F_{16}PcCu$  the transport of electrons was faster than the diffusion of ions as opposed to  $F_{64}PcCu$ . In this work, thin films of a new type of fluorinated phthalocyanine ( $F_{40}PcCu$ ) were prepared by physical vapor deposition. The dependence of the intermolecular coupling on the film thickness was analyzed by in situ UV/Vis spectroscopy. The electrochromic characteristics were studied by electrochemical and spectroelectrochemical measurements with an aqueous solution of *KCl* as electrolyte. The films provided a well-balanced, equally fast transport of electrons and ions. The optical absorption spectra revealed reversible changes of the films upon reduction with intercalation of the  $K^+$  counterions and re-oxidation with extraction of the counterions. Fast and stable electrochromic switching of the films was achieved over at least 200 cycles. For a 1:1 mixed film of  $F_{16}PcCu$  and  $F_{64}PcCu$  a similar situation could be achieved.

CPP 6.6 Mon 16:30 CPPp

**In Situ and In Operando KPFM Studies on Hexadecafluoro-Copper-Phthalocyanine ( $F_{16}PcCu$ ) in OFET to Access Electrical Contact Resistance and Energy Level Alignment** — ●PASCAL SCHWEITZER, CLEMENS GEIS, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, GERMANY

Contact resistances are considered the major limiter of performance of organic field effect transistors (OFET). Perfluorinated copper-phthalocyanine ( $F_{16}PcCu$ ) is a promising material as n-conductor to build complementary logical circuits. It is characterized by chemical stability under ambient conditions and a reasonably high charge carrier mobility. In this work, we used *in operando* Kelvin probe force microscopy under high vacuum to study the influence of contact resistances at the source and drain contacts on the OFET performance. Potentiometry at different applied external voltages revealed voltage drops at the interfaces to the source and drain metal contacts which allow for calculation of contact resistances. Thereby, the field-effect charge carrier mobility of  $F_{16}PcCu$  was corrected for contact effects. Significantly higher values were obtained. *In situ* KPFM during film growth on polycrystalline gold visualizes film formation and corre-

sponding shifts of energy levels confirming the existence of an injection barrier. We conclude, that tuning the energy level alignment and the interface effects to reduce contact resistances will lead to considerably improved performance of  $F_{16}PcCu$  in OFET.

CPP 6.7 Mon 16:30 CPPp

**Coupled organic-inorganic nanostructures (COINs) with mixed organic linker molecules** — ●FLORIAN GRASSL<sup>1</sup>, ALADIN ULLRICH<sup>1</sup>, AHMED E. MANSOUR<sup>3,4</sup>, SHAIMAA ABDALBAQI<sup>1</sup>, NORBERT KOCH<sup>3,4</sup>, ANDREAS OPITZ<sup>3</sup>, MARCUS SCHEELE<sup>2</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, Germany — <sup>2</sup>Institute for Physical and Theoretical Chemistry, University of Tübingen, Germany — <sup>3</sup>Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — <sup>4</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

COINs are composed of semiconducting inorganic nanoparticles and organic semiconductor molecules as ligands, which are covalently coupled to the surface of the nanoparticles [1]. A well-known organic ligand is 1,2-ethanedithiol (EDT) [2]; but it has the drawback of being very short as compared to the native oleic acid ligands. In this work we study the ligand Zinc  $\beta$ -tetraaminophthalocyanine (Zn4APc) [3], which has a desirable length comparable to oleic acid, but a low ligand exchange behaviour. To overcome this problem, a mixture of EDT and Zn4APc has been used. The binding of the ligands are compared by morphological, electronic, optical and electrical properties.

[1] M. Scheele, *Bunsen Magazin*, 2014, 4, 168

[2] J. Luther et al., *Nano Lett.*, 2008, 8, 3488

[3] J. Lauth et al., *Angew. Chem. Int. Ed.*, 2017, 56, 14061

CPP 6.8 Mon 16:30 CPPp

**Impact of thermal treatment and humidity exposure on surface concentration and work function of PEDOT:PSS thin films** — ●AMAN ANAND<sup>1,2</sup>, JOSE PRINCE MADALAIMUTHU<sup>1,2,3</sup>, MAXIMILIAN SCHAAL<sup>4</sup>, FELIX OTTO<sup>4</sup>, MARCO GRUENEWALD<sup>4</sup>, SHAHIDUL ALAM<sup>1,2</sup>, TORSTEN FRITZ<sup>4</sup>, ULRICH S. SCHUBERT<sup>1,2</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany — <sup>2</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — <sup>3</sup>Abbe School of Photonics, Friedrich Schiller University Jena, Albert-Einstein-Straße 6, 07745 Jena, Germany — <sup>4</sup>Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Poly (3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is the most common and successful commercial conductive polyelectrolyte in the field of optoelectronics. In the present work, we have investigated the impact of the thermal treatments and relative humidity during film casting or storage on the work function of PEDOT:PSS films made from various commercial formulations. We find clear trends between the processing conditions and absolute work function which could be associated with the metal ions on the surface of the films. As a conclusion, we can suggest suitable processing parameters for a wide range of formulations and targeted electronic properties

CPP 6.9 Mon 16:30 CPPp

**Compatible solution-processed interface materials for improving efficiency and prolonging the lifetime of organic solar cells** — ●ZHUO XU<sup>1,2</sup>, JOSE PRINCE MADALAIMUTHU<sup>1,2,3</sup>, JOSEF BERND SLOWIK<sup>1,2</sup>, RICO MEITZNER<sup>1,2</sup>, SHAHIDUL ALAM<sup>1,2</sup>, ULRICH S. SCHUBERT<sup>1,2</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany. — <sup>2</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany. — <sup>3</sup>Abbe School of Photonics, Friedrich Schiller University Jena, Albert-Einstein-Straße 6, 07745 Jena, Germany

The electron transport layer (ETL) in an organic solar cell is one of the main components that play a crucial role in the separation of charges, improving efficiency, and increasing the lifetime of the solar cells. Herein, solution-processed PBDTTT-CT: PC70BM based organic solar cells were fabricated using PDINO, Titanium Oxide (TiOx), and the mixture of PDINO and TiOx as an ETL. A power conversion efficiency (PCE) of 7.9% was achieved when a mixture of PDINO and TiOx was used as an ETL, which is one of the highest reported efficiency for halogen-free solvent processed PBDTTT-CT:PC70BM based polymer solar cells (PSCs). Furthermore, lower recombination,

higher exciton dissociation probability, and longer lifetime were observed from the same device that indicates the selectivity of ETL can effectively improve the performance and stability of the solar cells.

CPP 6.10 Mon 16:30 CPPp

**Observing Singlet Fission in Time-Energy-Momentum Space** — ●ALEXANDER NEEF<sup>1</sup>, SEBASTIAN HAMMER<sup>2</sup>, SAMUEL BEAULIEU<sup>1</sup>, SHUO DONG<sup>1</sup>, TOMMASO PINCELLI<sup>1</sup>, JULIAN MAKLAR<sup>1</sup>, MARTIN WOLF<sup>1</sup>, LAURENZ RETTIG<sup>1</sup>, JENS PFLAUM<sup>2</sup>, and RALPH ERNSTORFER<sup>1</sup> — <sup>1</sup>Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, 14195 Berlin, Germany — <sup>2</sup>Experimental Physics VI, Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Under suitable conditions, the optically excited singlet exciton in organic crystals can split into two triplet excitons, a process known as singlet fission (SF) [Michl, 2010]. Though extensively studied, the proposed mechanisms for SF [Berkelbach, 2013] have not yet been unambiguously verified experimentally.

By means of XUV time- and angle-resolved photoemission spectroscopy (trARPES) performed on crystals of the archetypical SF compounds pentacene and tetracene, we are - for the first time - able to directly observe the transient behavior of the excited singlet and triplet states ( $S_1$  and  $T_1$ ) in momentum space. This allows us to compare the  $S_1$  and  $T_1$  energies with respect to the dispersing valence band within one measurement, implying that the  $T_1$  energy is significantly smaller than previous estimates. Exploiting the multi-dimensionality of trARPES, we can furthermore decompose the excited states in pentacene by their unique signature in momentum space, thereby suggesting a strong mixing of charge-transfer (CT) states into  $S_1$  and hence a CT-mediated superexchange mechanism of SF.

CPP 6.11 Mon 16:30 CPPp

**Influence of solvent composition on optical and morphological properties of PTQ10:BTP-4F bulk heterojunctions** — ●LUKAS SPANIER, XINYU JIANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany

Organic solar cells have recently gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their production. However, their manufacture relies heavily on the use of halogenated solvents, as organic solar cells made with environmentally friendly solvents often suffer from major performance degradation. We investigate and compare the changes in morphology and the electro-optical behaviour of PTQ10:BTP-4F thin films processed from various solvents, utilising grazing-incidence X-ray scattering methods. We show the impact of solvent composition on the formation of polymer:non-fullerene acceptor bulk heterojunction films, affecting the resulting change in the performance of the organic solar cells.

CPP 6.12 Mon 16:30 CPPp

**Qualification of Thieno-Quinoxaline Based Polymers for Application in Non-Fullerene Organic Solar Cells** — ●MD MOIDUL ISLAM<sup>1,2</sup>, SHAHIDUL ALAM<sup>1,2</sup>, RICO MEITZNER<sup>1,2</sup>, CHRISTOS L. CHOCHOS<sup>3,4</sup>, ULRICH S. SCHUBERT<sup>1,2</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany — <sup>2</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — <sup>3</sup>Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece. — <sup>4</sup>Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece

Next-generation organic solar cells should not only be improved in performance but also should be environment-friendly throughout the production process. The processing of polymer-based solar cells with green solvents are highly desirable to make environmental friendly solar cells. In this study, we present bulk heterojunction polymer solar cells based on the thieno-quinoxaline based polymers blended with non-fullerene acceptor (NFA) in the non-halogenated solvent. Solar cells were prepared in conventional and inverted architecture, in order to investigate the material properties various spectroscopic measurements were performed in the pristine and blend films, as well as in the solutions. Finally, photovoltaic performances were investigated by different opto-electrical characterizations.

CPP 6.13 Mon 16:30 CPPp

**Simulation of light-induced exciton diffusion and quench-**

ing on SWCNTs — ●MANUEL ROMMEL<sup>1</sup>, RALPH KRUPKE<sup>1,2</sup>, and WOLFGANG WENZEL<sup>1</sup> — <sup>1</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, 76021 Karlsruhe — <sup>2</sup>Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt

The diffusion of excitons and charge carriers and the exciton loss processes like decay and quenching play an important role for the current characteristics in systems with light-induced charge carriers. A power-dependent photocurrent measurement on polymer-wrapped semiconducting single walled carbon nanotubes (SWCNT) has revealed a sub-linear scaling of the electric current with laser power.

Here, we present a modified Monte-Carlo-based simulation with a fixed timestep and a pulsed laser. It models the stochastic generation, diffusion, collision and quenching of excitons, electrons and holes in 1D. Our results show that there are two regimes depending on laser power. At low laser power, current scales linearly with laser power. For high laser power (which coincides with the onset of exciton-exciton-quenching), the exponent of the power dependence becomes 0.63, which is very close to the experimental value of  $0.59 \pm 0.08$ . Furthermore, we can show that even a perfectly symmetric 1D system, where both electrodes favor the same charge carrier, exhibits a photocurrent if the illumination is asymmetric. We also show that power law characteristics depend on the SWCNT length.

This gives an insight into diffusion in SWCNTs and highlights the importance of exciton-exciton-quenching in SWCNT devices.

CPP 6.14 Mon 16:30 CPPp

**In-situ sputter deposition of electrodes for non-fullerene organic photovoltaics application** — ●XINYU JIANG<sup>1</sup>, SIMON J. SCHAPER<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2,3</sup>, JONAS DREWES<sup>4</sup>, OLEKSANDR POLONSKYI<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Frank-Str. 1, Garching, Germany — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg, Germany — <sup>3</sup>KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — <sup>4</sup>Christian Albrechts-Universität zu Kiel, Materialverbunde Lehrstuhl, Materialwissenschaft Institut, Kaiserstr. 2, D-24143 Kiel, Germany — <sup>5</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Electrode quality of photovoltaic devices plays a very important role in device performance. The metal growth process directly influences the material density, electrical conductivity and interface contact of the electrode. For understanding the mechanism of aluminium cluster growth on non-fullerene organic solar cells, we use in-situ grazing-incidence small-angle X-ray scattering (GISAXS) to observe detailed information during the sputtering process. We find that the early stages of Al cluster growth on the non-fullerene active layers determine the later stages and strongly influence the percolation threshold. Furthermore, the cluster growth varies for active layers with an additional electron blocking layer. These findings are of great importance for improving the performance of the photovoltaic devices.

CPP 6.15 Mon 16:30 CPPp

**Sputter Deposition of Silver on Nanostructured PMMA-b-P3HT Copolymer Thin Films** — ●MARC GENSCHE<sup>1,2</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, CALVIN BRETT<sup>1,3</sup>, SIMON SCHAPER<sup>2</sup>, LUCAS KREUZER<sup>2</sup>, NIAN LI<sup>2</sup>, WEI CHEN<sup>2</sup>, SUZHE LIANG<sup>2</sup>, JONAS DREWES<sup>4</sup>, OLEKSANDR POLONSKYI<sup>4</sup>, THOMAS STRUNSKUS<sup>4</sup>, FRANZ FAUPEL<sup>4</sup>, PETER MÜLLER-BUSCHBAUM<sup>2,5</sup>, and STEPHAN ROTH<sup>1,3</sup> — <sup>1</sup>DESY, Hamburg, Germany — <sup>2</sup>TUM, München, Germany — <sup>3</sup>KTH, Stockholm, Sweden — <sup>4</sup>CAU, Kiel, Germany — <sup>5</sup>MLZ, München, Germany

Nanostructured polymer-metal-composite films demonstrate great perspectives for optoelectronic applications, e.g. as sensors or organic photovoltaics (OPV). To enhance properties of such devices the metal cluster self-assembly process needs to be understood. We correlate the emerging nanoscale morphologies with electronic properties and quantify the difference in silver growth, comparing the diblock copolymer template with its corresponding homopolymer thin film counterparts. In this contribution, we investigate the silver cluster morphology during the growth on a PMMA-b-P3HT diblock copolymer template. We applied with grazing incidence small-angle X-ray scattering (GISAXS) to observe the cluster formation. Our study reveals the selective wetting of silver on one of the polymer blocks and the influence of the template on the percolation behavior of the silver layer, which is measured with resistance measurements during the sputter deposition.

CPP 6.16 Mon 16:30 CPPp

**Memory effects in polymer brushes showing co-nonsolvency effects** — ●SIMON SCHUBOTZ<sup>1,2</sup>, PETRA UHLMANN<sup>1</sup>, ANDREAS FERY<sup>1,2</sup>, JENS-UWE SOMMER<sup>1,2</sup>, and GÜNTER K. AUERNHAMMER<sup>1,3</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — <sup>2</sup>Technische Universität Dresden, 01069 Dresden, Germany — <sup>3</sup>Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. Previous studies focused on the response of brushes which are entirely covered by a liquid. Here, we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes. We demonstrate that the wetting behavior depends on the wetting history of the polymer brush. We use Poly(N-isopropylacrylamide) (PNiPAAm) brushes and water and ethanol as good solvents. In water/ethanol mixtures, the brush thickness is a non-monotonous function of the ethanol concentration. The memory of brushes is tested by consecutively depositing drops of increasing size at the same position. Previously deposited drops induce changes in the brush that modifies the wetting behavior (advancing contact angle) of subsequent drops. We believe that the change in the contact angle is induced by adaptation like swelling of or liquid exchange in the brush due to the drop on top.

CPP 6.17 Mon 16:30 CPPp

**Quantification of Interfacial Fracture in Geometrically Confined Soft Elastomers by a Combined Analysis of Contact Force and Pressure** — ●HARES WAHDAT and ALFRED CROSBY — Polymer Science and Engineering Department, University of Massachusetts Amherst, Amherst, MA, USA

Interfacial fracture occurs in many different situations ranging from the failure of polymer adhesives to the growth of wounds in human skin. Commonly, interfacial fracture can be studied by inserting a needle into a soft material and apply positive pressure while recording images. The combination of pressure and corresponding images has revealed insight into the interfacial fracture properties of gels or biological tissues. Still, the need for recording images can complicate the study of non-transparent samples or in-vivo studies. Here, we present experiments, in which the pressure-change and the corresponding contact between a rigid probe in contact with micrometer-thin soft elastomers, were analyzed to quantify the critical strain energy release rate for interfacial fracture. The modeling of interfacial fracture does not require image recording, making our experiment and analysis suitable for quantitative studies of interfacial fracture in complicated systems such as biological tissues.

## CPP 7: Perovskites - organized by Eva M. Herzig (University of Bayreuth, Bayreuth)

Time: Tuesday 9:00–16:30

Location: CPPa

CPP 7.1 Tue 9:00 CPPa

**How do solvent molecules determine the electronic structure of halide perovskite precursors?** — ●ANA M. VALENCIA<sup>1</sup>, RICHARD SCHIER<sup>1</sup>, OLEKSANDRA SHARGAIEVA<sup>2</sup>, EVA UNGER<sup>2</sup>, and CATERINA COCCHI<sup>1</sup> — <sup>1</sup>Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof — <sup>2</sup>Helmholtz-Zentrum Berlin, HySPRINT Innovation Lab, Berlin

Hybrid metal-halide perovskites have been demonstrated as excellent

candidates for opto-electronic applications such as high-performing solar cells and light-emitting devices. The quality of the resulting materials, and hence their performance, strongly depends on the solution processing conditions. For this reason, it is of paramount importance to gain insight into their initial steps of formation of the solid-state materials. To do so, we investigate the inorganic building blocks of lead-iodide perovskites in DMSO solution. In order to mimic the initial steps of the perovskite nucleation, we consider PbI<sub>2</sub>(DMSO)<sub>4</sub>, Pb<sub>2</sub>I<sub>4</sub>(DMSO)<sub>6</sub>, and Pb<sub>3</sub>I<sub>6</sub>(DMSO)<sub>8</sub>, as model com-

pounds treated fully atomistically and quantum-mechanically in the framework of density-functional theory and many-body perturbation theory. Through the analysis of the computed molecular orbitals, optical spectra, and electron and hole densities we discuss and rationalize the role of electronic hybridization between solute and solvent, and the mechanisms that are responsible for the absorption and emission peaks observed in the experiments.

CPP 7.2 Tue 9:20 CPPa

**Solution-Processed Perovskite Solar Cells** — FLORIAN MATHIES<sup>1</sup>, GOPINATH PARAMASIVAM<sup>1</sup>, JANARDAN DAGAR<sup>1</sup>, and EVA UNGER<sup>1,2</sup> — <sup>1</sup>Helmholtz Zentrum Berlin — <sup>2</sup>Lund University, Sweden

Metal halide perovskites (MHP) are being intensively researched for solar energy conversion applications and are the best solution-processable solar cell technology to date. For scaling the technology, high throughput and material-efficient printing and coating techniques can be utilised to make larger area devices. We will here present our systematic approach translating successful processing strategies developed for spin-coating to slot-die coating and inkjet printing through in-depth rationalisation of MHP formation gained from in-situ optical monitoring. Depending on the composition of MHP precursors and solvents as well as process conditions and process quenching by e.g. an antisolvent, thin film formation proceeds via crystalline intermediate phases or directly into the perovskite phase. Optimisation of MHP precursors composition and processing conditions enabled us to recently achieve 22% power conversion efficiency in small area devices by spin-coating and 15% on large area mini-modules that are being further optimised in the near future. We are currently working on translating process conditions to obtain high quality perovskite thin films to scalable solution based deposition methods such as slot-die coating and inkjet printing. To date, we have demonstrated slot-die coating and inkjet printed small area devices with power conversion efficiencies > 15%.

CPP 7.3 Tue 9:40 CPPa

**In situ reflectometry and air flow control enables modeling of the drying process in blade coated hybrid perovskite solution films.** — SIMON TERNES<sup>1,2,3</sup>, TOBIAS BÖRNHORST<sup>3</sup>, JONAS A. SCHWENZER<sup>1</sup>, IHTAZ M. HOSSAIN<sup>1,2</sup>, ULI LEMMER<sup>1</sup>, PHILIP SCHARFER<sup>2,3</sup>, WILHELM SCHABEL<sup>3</sup>, BRYCE S. RICHARDS<sup>1,2</sup>, and ULRICH W. PAETZOLD<sup>1,2</sup> — <sup>1</sup>Light Technology Institute, Karlsruhe, Germany — <sup>2</sup>Institute of Microstructure Technology, Eggenstein-Leopoldshafen, Germany — <sup>3</sup>Institute of Thermal Process Engineering, Karlsruhe, Germany

In recent years, hybrid perovskite solar cells (PSCs) have been introduced to the field of thin-film photovoltaics, exhibiting not only a steep increase in power conversion efficiencies from 3.8% in 2009 to above 25% to date, but also opening the perspective toward low-cost, large-scale solution processing. However, in order to design industrial-scale printing machines for PSCs in an efficient manner, general modeling of the dynamic drying and crystallization processes in perovskite solution films is required. This modeling must extend beyond trail-and-error optimization and beyond the commonly used, non-scalable spin coating technique. In the work presented here, we demonstrate simultaneous exact drying control by a laminar air flow and in situ film thickness measurements by reflectometry on blade coated perovskite solution films. In this way, we derive a general model of the drying process in these solution films and correlate it with the evolving morphology, providing a strategy of optimal process transfer from spin coating to any industrial coating and drying technique.

CPP 7.4 Tue 10:00 CPPa

**Understanding the crystallization of solution processed, alloyed perovskites by multimodal characterization** — SHAMBHAVI PRATAP<sup>1,2</sup>, NOBUMICHI TAMURA<sup>2</sup>, ZHENGHAO YUAN<sup>3</sup>, ALASTAIR MACDOWELL<sup>2</sup>, NICOLA BARCHI<sup>4</sup>, JONATHAN SLACK<sup>2</sup>, CAROLIN SUTTER-FELLA<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Lehrstuhl für Funktionelle Materialien, TU München, 85748 Garching, Germany — <sup>2</sup>Advanced Light Source, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA — <sup>3</sup>Eberly College of Science, The Pennsylvania State University, State College, 16801, USA — <sup>4</sup>Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA

The crystallization behavior of solution processed hybrid plumbobalide perovskites is an ideal study to understand the formation of chemical alloys. Precursors corresponding to two different perovskites are mixed to serve as the precursor for an alloyed species. During crystallization, distinct crystalline species are isolated and characterized, as the equilibrium

between the complex precursor intermediates and perovskites is transformed to the crystalline product by annealing the structure. The evolution of chemical structures is temporally resolved and the transient structures are studied for their optoelectronic transformation by photoluminescence.

40 min. meet the speakers - break

Invited Talk

CPP 7.5 Tue 11:00 CPPa

**Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites** — FELIX DESCHLER — TU Munich

Metal-halide perovskites have emerged as promising semiconductors for optoelectronics, in which the soft-crystalline material structure leads to unexpected excitation dynamics, and for which the underlying physics remain unexplored. Unusually strong spin-orbit coupling was predicted to introduce Rashba-type state splitting in the electronic band structure of these materials, which is expected to affect recombination dynamics and spin-populations. It remains an open question, how dynamic changes in the material structure and electronic state populations control application-relevant electronic state nature and relaxation.

In my talk I will present how we use advanced optical spectroscopy to study the dynamics of optically-excited electronic state populations and crystal structure in functional hybrid perovskite semiconductors on ultrafast timescales. I will present results on mixed-cation mixed-halide bulk metal-halide perovskites, for which I will discuss how photodoping controls the properties and recombination of electronic states, and how these can enable highly-efficient optoelectronic devices and novel functionality. I will further discuss recent results on tracking the polaronic nature of excitation on ultrafast time-scales with ultrafast time-resolved diffraction experiments, from which we extract charge localization dynamics in real time.

CPP 7.6 Tue 11:40 CPPa

**Investigating MAPbI<sub>3</sub> Thin Film Formation during Spin Coating by Simultaneous in Situ Absorption and Photoluminescence Spectroscopy** — MIHIRSINH CHAUHAN<sup>1,2</sup>, YU ZHON<sup>1</sup>, KONSTANTIN SCHÖTZ<sup>1</sup>, BRIJESH TRIPATHI<sup>2</sup>, ANNA KÖHLER<sup>1</sup>, SVEN HUETTNER<sup>1</sup>, and FABIAN PANZER<sup>1</sup> — <sup>1</sup>University of Bayreuth, Bayreuth, Germany — <sup>2</sup>Pandit Deendayal Petroleum University, Gandhinagar, India

Until today, the two-step processing method represents an attractive route for the thin film formation of halide perovskites. However, a fundamental understanding about the film formation dynamics in case of spin coating methylammonium iodide (MAI) on PbI<sub>2</sub> has not been established yet. Here we apply in-situ optical spectroscopy during the two-step film formation of the model halide perovskite MAPbI<sub>3</sub> via spin coating. We identify and analyze in detail the optical features that occur in photoluminescence and corresponding absorption spectra during processing. We find that the film formation takes place in five consecutive steps, including the formation of a MAPbI<sub>3</sub> capping layer via an interface crystallization and the occurrence of an intense dissolution-recrystallization process. Consideration of confinement and self-absorption effects in the PL spectra, together with consideration of the corresponding absorption spectra allows to quantify the growth rate of the initial interface crystallization to be 13 nm/s for our processing conditions. We find the main dissolution recrystallization process to happen with a rate of 445 nm/s, emphasizing its importance to the overall processing.

CPP 7.7 Tue 12:00 CPPa

**Structural, optical and dielectric properties of Cs<sub>2</sub>AgBiBr<sub>6</sub>, a lead-free perovskite for photovoltaic applications** — MELINA ARMER<sup>1</sup>, MAXIMILIAN SIRT<sup>2</sup>, PATRICK DÖRFLINGER<sup>1</sup>, JULIAN HÖCKER<sup>1</sup>, THOMAS BEIN<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — <sup>2</sup>Ludwigs Maximilian University München, 81377 München

As conventional perovskite solar cells contain lead and therefore suffer toxicity and stability issues, finding alternative and stable lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, lead-free Cs<sub>2</sub>AgBiBr<sub>6</sub> single crystals have been synthesized using different solution based approaches, permitting a detailed characterization of the optical and structural properties of this material. The morphology and quality of the as grown crystals has been evaluated using scanning electron

microscopy (SEM), energy dispersive X-ray microscopy (EDX) and X-ray diffraction (XRD). The crystals have been characterized using steady-state and time-resolved photoluminescence (PL) spectroscopy. We observed PL in the visible region characterized by large PL lifetimes. Furthermore, the dielectric constant of  $\text{Cs}_2\text{AgBiBr}_6$  crystals has been measured at 9 GHz by time resolved microwave conductivity (TRMC). Using the obtained value of the dielectric constant the mobility of  $\text{Cs}_2\text{AgBiBr}_6$  thin films could be estimated using TRMC.

CPP 7.8 Tue 12:20 CPPa

**The Efficiency Potential of Neat Perovskite Films** — ●MARTIN STOLTERFOHT — Uni Potsdam

Perovskite photovoltaic (PV) cells have demonstrated power conversion efficiencies (PCE) that are close to those of monocrystalline silicon (m-Si) cells, however, in contrast to silicon PV, perovskites are not limited by Auger recombination. Nevertheless, compared to GaAs and m-Si devices, perovskite cells stand out by their significantly lower fill factors (FFs) which is due to a combination of resistive and non-radiative recombination losses. This necessitates a deeper understanding of the underlying loss mechanism and in particular the ideality factor of the cell. Here, by measuring the intensity (I) dependence of the external ( $V_{OC}$ ) and internal voltage (i.e. the quasi-Fermi level splitting, QFLS), we can quantify the transport resistance-free efficiency of the complete cell as well as the efficiency potential of any neat perovskite films with and without attached transport layers (TLs). Moreover, QFLS(I) measurements on different perovskite compositions allow to disentangle the impact of the interfaces and the perovskite surface on the non-radiative FF and  $V_{OC}$  loss. We find that potassium passivated quadruple cation perovskite films stand out by their exceptionally high implied PCEs of above 28% which could be readily achieved if charge collection losses and energy alignment issues are overcome. Finally, strategies are presented to reduce both the ideality factor and transport losses to push the FF to the thermodynamic limits.

**80 min. meet the speakers - break**

**Invited Talk**

CPP 7.9 Tue 14:00 CPPa

**Structural dynamics of halide perovskites via in-situ electron microscopy** — ●CHEN LI — Electron microscopy for Materials research (EMAT), University of Antwerp, Antwerp, Belgium

In-situ heating in electron microscopy is a powerful means of investigating phase changes in materials [1], and the focused electron probe in scanning transmission electron microscope (STEM) can also be used to stimulate the movement of atoms [2]. Here we apply such dynamic STEM to directly observe ion migration in both organic and inorganic halide perovskites. For instance, a phase transition from an orthorhombic  $\delta$ -phase to a cubic  $\alpha$ -phase in inorganic  $\text{CsPbI}_3$  perovskites has been tracked in atomic scale.

[1] C. Li, et. al., Secondary-phase-assisted grain boundary migration in  $\text{CuInSe}_2$ . *Phys. Rev. Lett.* 2020, 124, 095702

[2] C. Li, et. al., Column-by-column observation of dislocation motion in CdTe: dynamic scanning transmission electron microscopy, *Appl. Phys. Lett.* 2016, 109, 143107

CPP 7.10 Tue 14:40 CPPa

**The tetragonal to orthorhombic crystal phase transition in MAPI studied by time-resolved photoluminescence microscopy** — ●ALEXANDER BIEWALD<sup>1</sup>, NADJA GIESBRECHT<sup>1</sup>, RICHARD CIESIELSKI<sup>1</sup>, THOMAS BEIN<sup>1</sup>, PABLO DOCAMPO<sup>2</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>LMU München, Butenandstr. 11, 81377 Munich, GER — <sup>2</sup>Newcastle University, Newcastle upon Tyne, UK

Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22% [1]. Methylammonium lead iodide (MAPI) is prototypical for this material class of hybrid halide perovskite semiconductors and at the focal point of interest for a growing community in research and engineering. We investigated the diffusion properties for the orthorhombic and tetragonal phase using time-resolved photo-

luminescence (PL) microscopy before [2]. Now we focus on the PL dynamics at the phase transition. First, the phase transition is observed in temperature dependent PL spectra, which show the correlated decrease and rise of two spectrally distinct bands. This indicates the coexistence of both phases in a limited temperature range. Second, at the phase transition, which is found to vary between grains, diffusive transport suddenly stops and only reappears upon further cooling or heating, respectively. Our spatio-temporal studies provide detailed microscopic insights into the phase transition and its influence on the carrier dynamics in large crystal MAPI thin films.

[1] M.A.Green et al.,*Prog. Photovolt: Res. Appl.*,26,427-436,2018

[2] A. Biewald et al.,*ACS Appl. Mat. & Interfaces*,11,20838-20844,2019

CPP 7.11 Tue 15:00 CPPa

**Characterization of Perovskite Precursor Solutions in order to achieve High-Performance Solar Cells** — ●MARION FLATKEN<sup>1</sup>, NGA PHUNG<sup>1</sup>, ROBERT WENDT<sup>1</sup>, ARMIN HOELL<sup>1</sup>, and ANTONIO ABATE<sup>1,2</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin für Materialien und Energie (HZB) — <sup>2</sup>Department of Chemical, Materials and Production Engineering, University of Naples Federico II

Despite the current success of Perovskite Solar Cells, there are still open questions how to explain intrinsic parameters in terms of stability and general photovoltaic performance of varying perovskite compositions. Deeper knowledge in coordination chemistry of the perovskite itself is one key parameter to improve and control crystallization in the solution based fabrication. Using small angle scattering we can prove, that the coordination starts in the perovskite precursor solution and differs according to the perovskite composition. The observed colloidal structures are characterized via small angle neutron scattering (SANS) and is further compared to synchrotron based small angle x-ray scattering (SAXS). Based on nuclear magnetic resonance spectroscopy the chemical composition of the complexes can be revealed, which leads us to a possible starting mechanism for nucleation and growth in perovskite precursor solutions. In our work we compare the precursor solutions of  $\text{MAPbI}_3$  and  $\text{MAPbI}_3 \times \text{SrI}_2$  to a cesium containing triple cation perovskite solution, which is known to be a highly efficient and stable perovskite. Observed differences and similarities might give one reason for the divergence in photovoltaic properties of the respective full device solar cells.

CPP 7.12 Tue 15:20 CPPa

**Thermal decomposition dynamics of lead halide perovskite thin films** — THOMAS BURWIG, KARL HEINZE, ROLAND SCHEER, and ●PAUL PISTOR — MLU Martin-Luther-Universität Halle-Wittenberg

Despite the remarkable progress of lead halide perovskites, their low stability severely limits practical applications. To understand degradation pathways and pinpoint optimal compositions in terms of stability is therefore of utmost importance. Here we investigate the thermal stability of lead halide perovskite thin films grown by co-evaporation and analyze their thermal decomposition at elevated temperatures. Our approach allows to investigate the thermal decomposition by time-resolved in situ X-ray diffraction inside the vacuum growth chamber, without exposing the perovskite thin film to moisture or ambient air at any time. By applying fixed temperature ramps of 3-4 K/min. , we compare the onset of decomposition for a variety of different  $\text{ABX}_3$  compositions and explore perovskites throughout the compositional space with  $\text{A}=\text{MA,FA,Cs}$ ;  $\text{B}=\text{Pb,Sn,(Ag,Bi)}$  and  $\text{X}=\text{I,Br,Cl}$ . We find an increasing decomposition temperature for the series  $\text{MAPbCl}_3$  -  $\text{MAPbI}_3$  -  $\text{MAPbBr}_3$ , where the perovskite decomposes via degassing of MAX. The cation variation shows increased stability for  $\text{CsPbBr}_3$  over  $\text{FAPbBr}_3$  and  $\text{MAPbBr}_3$ , mainly due to the increased sublimation temperature of CsX, which is even higher than that of  $\text{PbX}_2$ . Finally, for the case of the most common and less stable  $\text{MAPbX}_3$  perovskites, a series of time-resolved degradation experiments at constant temperatures provides detailed insights into the degradation kinetics of these materials.

**50 min. meet the speakers - break**

## CPP 8: Complex Fluids - organized by Christine M. Papadakis (Technical University of Munich, Garching) (joint session CPP/DY)

Time: Tuesday 9:00–16:30

Location: CPPb

**Invited Talk**

CPP 8.1 Tue 9:00 CPPb

**Polymer Micelles with Crystalline Cores: confinement effects, molecular exchange kinetics and mechanical response** — NICO KOENIG<sup>1</sup>, LUTZ WILLNER<sup>2</sup>, and •REIDAR LUND<sup>1</sup> — <sup>1</sup>Department of Chemistry, University of Oslo, Postboks 1033 Blindern, 0315 Oslo, Norway. — <sup>2</sup>Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS,

Partially crystalline, self-assembling systems with multiple components are omnipresent in nature with living cells as a prominent example. Here we study micelles formed by self-assembly of a series of well-defined n-alkyl-(polyethylene oxide) (C<sub>n</sub>-PEO) polymers in aqueous solutions [1]. Using small-angle X-ray/neutron scattering (SAXS/SANS), densimetry and differential scanning calorimetry (DSC), we show that the n-alkane exhibit a first-order phase transition in the micellar cores, but with reduced melting points accurately described by the Gibbs-Thomson equation [2]. The effect of core crystallinity on the molecular exchange kinetics is investigated using time-resolved SANS (TR-SANS) [3-9]. We show that the melting transition is cooperative in the confined micellar core, whereas the exchange process is decoupled and unimeric in nature. [9] Telechelic polymers based on C<sub>n</sub>-PEO-C<sub>n</sub> forms clustered micelles and hydrogels composed of interconnected micelles at higher concentrations.[10] The results show that, contrary to regular micelles, the kinetics occurs in a multistep process involving a novel collision-induced single-molecule exchange mechanism.[11] Moreover exchange kinetics directly controls the mechanical response of hydrogels through the bond life time [12]

CPP 8.2 Tue 9:40 CPPb

**Foams stabilized by PNIPAM microgels** — •MATTHIAS KÜHNHAMMER, CHRISTIAN APPEL, and REGINE VON KLITZING — Technical University of Darmstadt, Department of Physics, Soft Matter at Interfaces, 64287 Darmstadt, Germany

Cross-linked, short-chained poly-N-isopropylacrylamide (NIPAM) polymers have been in the focus of numerous studies in the past years and are still being discussed very actively in the context of multiple possible applications, because of their ability to respond to external stimuli. Because of their amphiphilic character, PNIPAM microgels can be used to stabilize dispersions like emulsions or foams.

In this contribution microgel stabilized foams are investigated. These foams are very stable at temperatures below the volume phase transition temperature (VPTT) of NIPAM and can be destabilized by increasing the temperature above the VPTT. The structure of the microgels inside the foam lamellae is investigated with neutron scattering. These results are compared to the organization of microgels at a single gas / water interface, which is studied with Langmuir isotherms and X-ray reflectivity.

Finally, these findings are related to macroscopic properties of the foams, namely foamability and foam stability.

CPP 8.3 Tue 10:00 CPPb

**Functional, responsive microgels enlightened with super-resolution fluorescence microscopy** — •DOMINIK WÖLL, LAURA HOPPE ALVAREZ, ERIC SIEMES, ASHVINI PUROHIT, and SILVIA CENTENO BENIGNO — Institut für Physikalische Chemie, RWTH Aachen University, Landoltweg 2, 52074 Aachen

The elucidation of the structure and functionalization of materials in the sub-micron range is a key to their further development and application. Microgels are a class of such soft materials with high potential for multiple fields. Several groups have learnt to functionalize and structure microgels in sophisticated ways, but the evaluation of a successful functionalization or the envisioned properties are often limited by the ways of analysis and visualization. The development of modern super-resolved fluorescence microscopy methods opened up new ways of nanoscopic visualization that had not been possible previously due to the diffraction limit of light prohibiting spatial resolution beyond approx. 200 nm. In my contribution, the possibilities to elucidate shape and functionalization, to visualize single cross-linker positions and to address local polarity in microgels with 3D super-resolution fluorescence imaging will be discussed, and ways presented to address and answer scientific questions in soft matter science.

40 min. meet the speakers - break

**Invited Talk**

CPP 8.4 Tue 11:00 CPPb

**Dynamic behaviour of anisotropic magnetic particles in suspensions** — •SOFIA KANTOROVICH — University of Vienna — Ural Federal University

Stable dispersions of magnetic colloidal particles with sizes ranging from nanometers to couple of microns have been actively studied for several decades and the interest to them seems to keep growing. Such an attention to these systems is paid because of several reasons: they are biocompatible, can be remotely controlled by external magnetic fields and new synthesis techniques enable a rich variety of particle morphologies. In classical magnetic fluids with spherical poly-disperse nanoparticles, dominating dipolar interactions typically limit the structural complexity of their aggregates to linear arrangements, namely chains, rings and branched structures. In this contribution I will show, how to either alter the shape of magnetic particles or their internal structure in order to extend dramatically the topology and properties of their suspensions. In particular I will focus on magnetic cubes, magnetic Janus particles, soft magnetic colloids and magnetically anisotropic nanoparticles. I will show how lattices, branched clusters of staggered chains, compact clusters, linear chains, and non aggregated configurations can be formed and interconverted reversibly in a controlled way. I will also discuss how adding an active component to magnetically anisotropic particles leads to unique properties. The results gathered in this presentation demonstrate that fundamentally new possibilities for responsive magnetic materials can arise when we step away from conventional dipolar hard spheres.

CPP 8.5 Tue 11:40 CPPb

**Graphical Magnetogranulometry** — •INGO REHBERG, REINHARD RICHTER, and STEFAN HARTUNG — Bayreuth University

The dipole strength of magnetic particles in a colloidal suspension can be obtained by a graphical rectification of the magnetization curves based on the inverse Langevin function. The method [1] yields the arithmetic and the harmonic mean of the particle distribution. It has an advantage compared to the fitting of magnetization curves to some appropriate mathematical model: It does not rely on assuming a particular distribution function of the particles.

[1] Measuring magnetic moments of polydisperse ferrofluids utilizing the inverse Langevin function, Ingo Rehberg, Reinhard Richter, Stefan Hartung, and Niklas Lucht, Birgit Hankiewicz, and Thomas Friedrich, Phys. Rev. B 100, 134425 (2019).

CPP 8.6 Tue 12:00 CPPb

**Phase Behavior of Charged Magnetic Nanoplatelets**

— •MARGARET ROSENBERG<sup>1</sup> and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>Department of Physics, University of Vienna, Austria — <sup>2</sup>Department of Mathematical Physics, Ural Federal University, Russia

Recent decades have seen the emergence of a new branch of science, magnetic soft matter, fueled by the advances in synthesis techniques, which have also made a wide variety of anisotropic magnetic colloidal nanoparticles available. Colloidal anisotropy can be used as an effective control parameter to tune both self-assembly scenarios and thermodynamic, rheological and phase behavior of dipolar (magnetic) soft matter. For instance, magnetic nanoplatelets can form macroscopic ferromagnetic phases at room temperature. Although the phase behavior of a system hard-core platelets is well known, the influence of the magnetic dipole moment and electrostatic repulsion on suspensions of magnetic platelets is not yet fully understood. We use MD simulations to recreate such a system. The colloidal particles are modelled by charged soft spheres, with a central dipole possessing a magnetic moment of a constant length, permanently oriented perpendicular to the platelet surface. In order to investigate the self-assembly and structural properties of the platelets, we vary the amplitude of an applied magnetic field and the magnetic dipole. We analyze at which electrostatic conditions the system exhibits self-assembly or/and field alignment, based on RDFs, structure factors parallel and perpendicular to the field and extensive cluster analysis.

CPP 8.7 Tue 12:20 CPPb

**Magnetically Functionalized Star Polymers in Equilibrium and under Shear** — ●GERHARD KAHL<sup>1</sup>, DAVID TONEIAN<sup>1</sup>, and CHRISTOS N. LIKOS<sup>2</sup> — <sup>1</sup>Institut für Theoretische Physik, TU Wien — <sup>2</sup>Fakultät für Physik, Universität Wien

Star polymers are macromolecules consisting of a central site, attached to which are a number  $f$  of linear polymer chains, called arms. Depending on the chemical composition of the arms, the polymer stars exhibit intriguing features, both in isolation and in concentrated solution.

We present star polymers with magnetically functionalized end groups as a novel polymeric system whose morphology, self-aggregation and orientation can easily be tuned by exposing these macromolecules simultaneously to an external magnetic field and to shear forces within a channel. Our investigations are based on a specialized simulation technique which faithfully takes into account the hydrodynamic interactions of the surrounding, Newtonian solvent. We find that the combination of magnetic field (including both strength and direction) and shear rate controls the mean number of magnetic clusters, which in turn is largely responsible for the static and dynamic behavior. While some properties are similar to comparable non-magnetic star polymers, others exhibit novel phenomena; examples of the latter include the breakup and reorganization of the clusters beyond a critical shear rate and a strong dependence of the efficiency with which shear rate is translated into whole-body rotations on the direction of the magnetic field.

CPP 8.8 Tue 12:40 CPPb

**Structural details of polymer grafted nanoparticles: Insights from coarse-grained molecular dynamics simulations** — ●JIARUL MIDYA<sup>1</sup>, MICHAEL RUBINSTEIN<sup>2</sup>, SANAT K. KUMAR<sup>3</sup>, and ARASH NIKOUBASHMAN<sup>1</sup> — <sup>1</sup>Johannes Gutenberg University of Mainz, Mainz, Germany — <sup>2</sup>Duke University, Durham, United States — <sup>3</sup>Columbia University, New York, United States

Polymer grafted nanoparticles (GNPs) are promising materials with a wide range of applications in drug delivery, gas separation, photonic and electric materials. In this work, the structural properties of GNPs are studied via coarse-grained molecular dynamics simulations. We systematically vary the degree of polymerization at fixed grafting density, and study in detail the shape and size of the GNPs, the interpenetration between the grafted polymers and their conformations. We then compare these properties to the ones of pure polymer melts to assess the effect of confinement. We observe that the amount of chain-sections in the interpenetration zone is proportional to the length of the grafted chains,  $N_g$ , whereas, the brush height follows a power-law like behavior  $h \sim N_g^\alpha$ , where exponent  $\alpha$  decreases from a value close to one to the limiting value of 1/3 with the increase of  $N_g$ . To understand the scaling behavior of  $h$  we provide an empirical form, involving the length of the grafted polymers and the core size of the GNPs, which explains our simulation results.

60 min. meet the speakers - break

CPP 8.9 Tue 14:00 CPPb

**Charge regulation radically modifies electrostatics in membrane stacks** — ●ARGHYA MAJEE<sup>1</sup>, MARKUS BIER<sup>1,2</sup>, RALF BLOSSEY<sup>3</sup>, and RUDOLF PODGORNİK<sup>4</sup> — <sup>1</sup>MPI for Intelligent Systems, Stuttgart & University of Stuttgart, Germany — <sup>2</sup>University of Applied Sciences, Würzburg-Schweinfurt, Germany — <sup>3</sup>University of Lille, CNRS, UMR8576 UGSF, France — <sup>4</sup>CAS & KAVLI Institute of Theoretical Sciences, Beijing

Motivated by biological membrane-containing organelles in plants and photosynthetic bacteria, we study charge regulation in a model membrane stack [1]. Considering (de)protonation as the simplest mechanism of charge equilibration between the membranes and with the bathing environment [2], we uncover a symmetry-broken charge state in the stack with a quasiperiodic effective charge sequence. In the case of a monovalent bathing salt solution, our model predicts complex, inhomogeneous charge equilibria depending on the strength of the (de)protonation reaction, salt concentration, and membrane size. Our results shed light on the basic reorganization mechanism of thylakoid membrane stacks.

References:

- [1] A. Majee, M. Bier, R. Blossey, and R. Podgornik, *Phys. Rev. E* **100**, 050601(R) (2019).  
[2] A. Majee, M. Bier, and R. Podgornik, *Soft Matter* **14**, 985 (2018).

CPP 8.10 Tue 14:20 CPPb

**Emulsion destabilisation by squeeze flow** — ●RIANDE DEKKER, ANTOINE DEBLAIS, and DANIEL BONN — Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

There is a large debate on the destabilisation mechanism of emulsions. We present a simple technique using mechanical compression to destabilise oil-in-water emulsions while at the same time confocal microscopy allows to visualise the mechanism directly. Upon compression of the emulsion, the continuous aqueous phase is squeezed out, while the dispersed oil phase progressively deforms from spherical to honeycomb-like shapes. The liquid films that separate the oil droplets are observed to thin and break at a critical oil/water ratio, leading to coalescence events that destabilise the emulsion. The destabilisation occurs like an avalanche propagating through the system. Local rearrangements occur after the first destabilisation due to the first coalescence event. The films participating in the cascade are the finest ones.

CPP 8.11 Tue 14:40 CPPb

**Impact of hydrogen bonding strength on the structure and dynamics of supramolecular PEO** — ●ANA BRÁS<sup>1</sup>, ANA ARIZAGA<sup>1</sup>, UXUE AGIRRE<sup>1</sup>, MARIE DORAU<sup>1</sup>, PATRICIA BACH<sup>1</sup>, JUDITH E. HOUSTON<sup>2,3</sup>, AUREL RADULESCU<sup>3</sup>, MARGARITA KRUTEVA<sup>4</sup>, and ANNETTE M. SCHMIDT<sup>1</sup> — <sup>1</sup>UzK, Cologne, Germany — <sup>2</sup>ESS, Lund, Sweden — <sup>3</sup>FZJ, Garching, Germany — <sup>4</sup>FZJ, Jülich, Germany

In this work we investigate supramolecular poly(ethylene oxide) (PEO) oligomers at the entanglement molar mass (Me) with different hydrogen bonding end groups, such as diaminotriazine (Dat) and thymine-1-acetic acid (Thy), as well as 2-ureido-4[1H]-pyrimidinone (Upy). Small angle scattering and rheology were combined to study the influence of different end-groups association strength as Upy is highly self-associative in comparison to the heterocomplementary pair Thy/Dat. Results on the structure provide insight into the underlying molecular mechanisms and reveal that while Upy-terminated chains phase segregate, forming network-like systems, the Thy/Dat pair-terminated system self-assemble to linear chains, thereby increasing the effective chain length. Moreover, rheological measurements also reveal differences in the viscoelastic response as Upy-terminated chains exhibit an extended rubbery plateau, typical of networks, and the pair Thy/Dat presents a Newtonian fluid behaviour. Remarkably, albeit both systems show end-group association, different hydrogen bonding species influence the type of associates. Acknowledgements: DFG for a research grant (BR5303) and Prof. Dr. D. Richter, Prof. Dr. R. Strey and Dr. Wim Pyckhout-Hintzen for fruitful discussions.

CPP 8.12 Tue 15:00 CPPb

**Structural characterization and rheology of biocompatible wormlike micelles - comparing experiment and theory** — ●BENJAMIN VON LOSPICH<sup>1,2</sup>, SABINE H. L. KLAPP<sup>2</sup>, and MICHAEL GRADZIELSKI<sup>1</sup> — <sup>1</sup>Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 124, D-10623 Berlin — <sup>2</sup>Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin

Wormlike micelles exhibit a unique viscoelastic behaviour, which has been investigated intensely in the past decades by experimentalists and theoreticians [1,2]. Within our studies we explore the self-assembled structures and the flow behaviour of biocompatible wormlike micelles, which are a mixture of a short-chained C<sub>8</sub> cationic surfactant and the salts of long-chained C<sub>18</sub> to C<sub>22</sub> omega-9 fatty acids. The variation of the omega-9 fatty acids yields a change in thickness of the micelles, which strongly influences the flowing properties of the system. To characterize the size distribution and the relaxation time of the micellar solutions we use neutron scattering, rheology and electric birefringence. The obtained experimental results are then quantitatively compared to an established theoretical model describing the dynamics of micelles under shear. The model links mechanical properties such as stress to structural quantities like alignment or micellar length [3].

[1] C. Dreiss, *Soft Matter* **3**, 956, (2007)[2] P. D. Olmsted, *Rheo. Acta* **47**, 283, (2008)[3] B. v. Lospichl, S. H. L. Klapp, *Phys. Rev. E* **98**, 042605, (2018)

CPP 8.13 Tue 15:20 CPPb

**Light driven passive and active motion of colloidal particles** — ●POOJA ARYA, DAVID FELDMANN, and SVETLANA SANTER — University of Potsdam, Potsdam, Germany



We report on how one can manipulate an ensemble of colloidal particles trapped at a solid/liquid interface during irradiation with light of different wavelengths. The colloids are dispersed in an aqueous solution of photosensitive azobenzene containing cationic surfactant, which can photo-isomerize from trans to cis state under irradiation with light of appropriate wavelength. When focused light is applied, light-driven diffusioosmotic (LDDO) flow is generated at the solid/liquid interface resulting in a passive motion of particles within this flow. Utilizing the same LDDO mechanism one can also induce active motion of porous particles. Here the radially directed flow is generated by and around a

single porous colloid when it is irradiated with either UV or blue light. This results in either mutual long-range diffusioosmotic repulsion of the particles or in even self-propelled motion when the colloids are turned into a Janus-like shape. Here, we discuss how to extend of passive and active motion of colloidal particles depends on the irradiation conditions such as wavelengths and intensities of light.

1.\*Feldmann, D.; Maduar S.R.; Santer, M.; Lomadze, N.; Vinogradova, O.I.; Santer, S., *Scientific Reports* 6 (2016) 36443

50 min. meet the speakers - break

## CPP 9: Focus Phase Separation in Biological Systems I (joint session BP/CPP)

Time: Tuesday 9:00–11:00

Location: BPC

CPP 9.1 Tue 9:00 BPC

**Intranuclear Phase Separation of a Chromatin Scaffolding Protein** — ●DAVIDE MICHIELETTI<sup>1</sup>, MATTIA MARENDA<sup>1</sup>, DAVID ZWICKER<sup>2</sup>, and JAN KIRSCHBAUM<sup>2</sup> — <sup>1</sup>University of Edinburgh — <sup>2</sup>Max Planck Institute for Dynamics and Self-Organization

The formation and regulation of phase separated condensates is now widely seen in vitro and cytoplasm, but far more challenging to observe and test in the cell nucleus. In this talk I will present recent work on an abundant nuclear RNA-binding protein called Scaffold Attachment Factor A, or SAF-A, that regulates chromatin decompaction at transcriptionally active loci through its interaction with RNA. Here I show that the intrinsically disordered RNA binding domain of SAF-A \* known as an RGG domain – undergoes phase separation upon transcriptional inhibition and that the size of the condensates can be controlled by tuning the amount arginine/lysine residues in the RGG domain. By expressing a longer, and closer to native, SAF-A domain we observe that the phase separation is suppressed. To explain our findings, we propose an equilibrium model in which a slowly diffusing RNA substrate can sequester RGG fragments; upon transcriptional inhibition the freed up fragments can undergo phase separation via weak self-interactions.

CPP 9.2 Tue 9:20 BPC

**Quantitative phase microscopy enables precise and efficient determination of biomolecular condensate composition** — ●PATRICK M MCCALL<sup>1,2</sup>, K KIM<sup>3,4</sup>, AW FRITSCH<sup>1</sup>, JM IGLESIAS-ARTOLA<sup>1</sup>, LM JAWERTH<sup>1,2</sup>, J WANG<sup>1</sup>, M RUER<sup>1</sup>, A POZNYAKOVSKIY<sup>1</sup>, J PEYCHL<sup>1</sup>, J GUCK<sup>3,4</sup>, S ALBERTI<sup>3</sup>, AA HYMAN<sup>1</sup>, and J BRUGUÉS<sup>1,2</sup> — <sup>1</sup>MPI-CBG, Dresden — <sup>2</sup>MPI-PKS, Dresden — <sup>3</sup>TU Dresden — <sup>4</sup>MPI Science of Light

Many cellular processes rely on condensed macromolecular phases termed biomolecular condensates. Despite progress in measurements and theoretical descriptions of several condensate properties, an understanding of their most basic feature, composition, remains elusive. Here we combined quantitative phase microscopy and sessile droplet physics to measure the shape and composition of individual model condensates. This technique requires 1000-fold less material than traditional approaches, achieves a precision of better than 2 %, and does not rely on fluorescent tags, which we show can significantly alter phase behavior. The protein concentrations measured in three model condensates span a broad range, from 80 to 500 mg/ml, pointing to a natural diversity in condensate composition specified by protein sequence. We report salt- and temperature-dependent binodals as well as time-resolved measurements revealing that PGL3 condensates undergo a contraction-like process during aging. This leads to doubling of the internal protein concentration coupled to condensate shrinkage. We anticipate that this new approach will enable understanding the physical properties of biomolecular condensates and their function.

CPP 9.3 Tue 9:40 BPC

**Quantitative Theory for the Diffusive Dynamics of Liquid Condensates** — ●LARS HUBATSCH<sup>1,2</sup>, LOUISE M JAWERTH<sup>1,2</sup>, CELINA LOVE<sup>2</sup>, JONATHAN BAUERMANN<sup>1</sup>, STEFANO BO<sup>1</sup>, T-Y DORA TANG<sup>2</sup>, ANTHONY A HYMAN<sup>2</sup>, and CHRISTOPH A WEBER<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — <sup>2</sup>Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

To unravel the biological functions of membraneless liquid condensates it is crucial to develop a quantitative understanding of the physics underlying their dynamics. Key properties of such condensates are diffusion and exchange of material with their environment. Experimentally, such diffusive dynamics are typically probed through the direct observation of the individual or collective motion of fluorescently labelled molecules. However, to date we lack a physics-based quantitative framework for the dynamics of labeled condensate components. Here, we derive the corresponding theory, building on the physics of phase separation, and quantitatively validate this framework via experiments. We show that using our theory we can precisely determine diffusion coefficients inside liquid condensates via a spatio-temporal analysis of fluorescence recovery after photobleaching (FRAP) experiments. We showcase the accuracy and precision of our approach by considering space and time resolved data of protein condensates and two different coacervate systems. Strikingly, our theory can be used to determine the diffusion coefficient in the dilute phase and the partition coefficient, purely based on fluorescence measurements in the droplet.

CPP 9.4 Tue 10:00 BPC

**Interactions of droplets with polymer networks at the mesh and continuum scale** — ●THOMAS J BOEDDEKER<sup>1</sup>, ESTEFANIA VIDAL<sup>2</sup>, KATHRYN A ROSOWSKI<sup>1</sup>, DAVID ZWICKER<sup>2</sup>, and ERIC R DUFRESNE<sup>1</sup> — <sup>1</sup>ETH Zurich, Zurich, Switzerland — <sup>2</sup>MPI DS, Göttingen, Germany

Phase-separation of biomolecules in cells takes place in a complex environment crossed by multiple filaments of the cytoskeleton or chromatin. Interactions between the emerging protein droplets and filaments take place over different length scales and may lead to motion and deformation of both network and droplet. In this shared talk, Thomas presents experimental work on the interactions of stress granules, a phase-separated protein-RNA droplet in the cytosol, with the heterogeneous microtubule network at the mesh scale. Inspired by observations in the cell, we then turn to synthetic gels where elastic effects produce ripening in stiffer materials leading to a dissolution front. Estefania presents a theoretical framework for the observed ripening in gradients of network stiffness at the continuum scale. Our combined results present an initial approach to understand the complex interactions throughout phase separation in an elastic network.

30 min. Meet the Speaker

## CPP 10: Active Matter 1 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/ CPP)

Time: Tuesday 9:30–10:30

Location: DYa

CPP 10.1 Tue 9:30 DYa

**Swirl formation of active colloids near criticality** — ●ROBERT C. LÖFFLER<sup>1</sup>, TOBIAS BÄUERLE<sup>1</sup>, MEHRAN KARDAR<sup>2</sup>, CHRISTIAN M. ROHWER<sup>3</sup>, and CLEMENS BECHINGER<sup>1</sup> — <sup>1</sup>FB Physik, Universität Konstanz, Germany — <sup>2</sup>Dep. Physics, MIT, Cambridge, MA, USA — <sup>3</sup>Dep. Mathematics, University of Cape Town, South Africa

Animal groups like flocks of birds or schools of fish normally show a high degree of order. Yet they are also responsive to external factors in order to optimize nutrition and avoid predation. Various observations of such responsiveness have led to the assumption that those systems represent a state of order close to a critical point.

In our experiments, we use light-responsive active Brownian particles (ABPs) to which we can apply individual torques in a feedback controlled system to study such behavioral rules. Through the variation of a single parameter in our interaction model based on information about a particles local neighbors, we observe a continuous phase transition in the collective motion of the group: The ABPs transition from a disordered swarm to a stable swirl (i.e. milling, vortex-like state). Being able to continuously change our control parameter we observe a critical point with explicit bifurcation dynamics in the rotational order parameter and critical slowing down, as well as hysteresis in the symmetry-breaking regime of the control parameter. Observation of such critical behavior in simple models not only allows for more insight in complex animal behavior but also helps with designing future rules for collective tasks in robotic or other autonomous systems.

Bäuerle *et al.*, Nat. Comm. **11**, 2547 (2020); Löffler *et al.* (in review).

CPP 10.2 Tue 9:50 DYa

**A particle-field approach bridges phase separation and collective motion in active matter** — ●ROBERT GROSSMANN<sup>1</sup>, IGOR ARANSON<sup>2</sup>, and FERNANDO PERUANI<sup>3</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — <sup>2</sup>Department of Chemistry, Pennsylvania State University, University Park (PA), United States of America — <sup>3</sup>Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université, Cergy-Pontoise, France

Linking seemingly disconnected realms of active matter – active phase-

separation of repulsive discs and collective motion of self-propelled rods – is a major contemporary challenge. We present a theoretical framework based on the representation of active particles by smoothed continuum fields which brings the simplicity of alignment-based models, enabling an analytical analysis, together with more realistic models for self-propelled objects including their steric, repulsive interactions. We demonstrate on the basis of the collision kinetics how nonequilibrium stresses acting among self-driven, anisotropic objects hinder the emergence of motility-induced phase separation and facilitate orientational ordering. Moreover, we report that impenetrable, anisotropic rods are found to form polar, moving clusters, whereas large-scale nematic structures emerge for soft rods, notably separated by a bistable coexistence regime. Thus, the symmetry of the ordered state is not dictated by the symmetry of the interaction potential but is rather a dynamical, emergent property of active systems. This theoretical framework can represent a variety of active systems: cell tissues, bacterial colonies, cytoskeletal extracts or shaken granular media.

CPP 10.3 Tue 10:10 DYa

**A Quantitative Kinetic Theory of Flocking in Dry Active Matter Including a Three Particle Closure** — ●RÜDIGER KÜRSTEN and THOMAS IHLE — Institut für Physik, Universität Greifswald, Germany

We consider aligning self-propelled point particles in two dimensions. Their motion is given by generalized Langevin equations, however, the qualitative behavior is as for the famous Vicsek model. We develop a kinetic theory of flocking beyond mean field. In particular, we take into account the full pair correlation function. We find excellent quantitative agreement of those pair correlations with direct agent-based simulations within the disordered regime. Furthermore we use a closure relation to incorporate the spatial correlations of three particles. In that way we achieve good quantitative agreement of the onset of flocking with direct simulations. Compared to mean field theory, the flocking transition is shifted significantly towards lower noise because angular correlations favor disorder.

## CPP 11: Active Matter 2 - organized by Carsten Beta (Potsdam), Andreas Menzel (Magdeburg) and Holger Stark (Berlin) (joint session DY/BP/ CPP)

Time: Tuesday 11:00–13:00

Location: DYa

CPP 11.1 Tue 11:00 DYa

**Mesoscale turbulence and dynamical clustering in active polar fluids** — ●VASCO MARIUS WORLITZER<sup>1</sup>, GIL ARIEL<sup>2</sup>, AVRAHAM BE'ER<sup>3</sup>, HOLGER STARK<sup>4</sup>, MARKUS BÄR<sup>1</sup>, and SEBASTIAN HEIDENREICH<sup>1</sup> — <sup>1</sup>Department of Mathematical Modelling and Data Analysis, Physikalisch-Technische Bundesanstalt, Abbestrasse 2-12, 10587 Berlin — <sup>2</sup>Department of Mathematics, Bar-Illan University, Ramat Gan 52000, Israel — <sup>3</sup>Zuckerberg Institute for Water Research of the Negev, Sede Boqer Campus 84900 Midreshet Ben-Gurion, Israel — <sup>4</sup>Institute of Theoretical Physics, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin

Bacterial suspensions are fascinating examples for active polar fluids which exhibit large scale collective behavior ranging from polar and disordered states to so-called mesoscale turbulence and vortex lattices. Previous approaches take into account the self-propulsion of bacteria and an effective polar-alignment interaction but assume for simplicity a constant density. Comparison with experiments showed that this modelling approach is successful, to some extent, in a relatively narrow regime corresponding to wild-type swarms in which density is indeed approximately constant and velocity distributions are Gaussian. We seek a unified model that can explain the observed phenomena across the entire phase space of swarming bacteria. To this end, we present a continuum model that allows variations in density. The model predicts new dynamical regimes, such as mixed states with coexisting vortex patterns and dynamical clusters, obeying anomalous statistics, similar to experimental observations.

CPP 11.2 Tue 11:20 DYa

**Rewarding cargo-carrier interactions: cell-mediated particle transport** — ●VALENTINO LEPRO<sup>1,2</sup>, ROBERT GROSSMANN<sup>1</sup>, OLIVER NÄGEL<sup>1</sup>, STEFAN KLUMPP<sup>3</sup>, REINHARD LIPOWSKY<sup>2</sup>, and CARSTEN BETA<sup>1</sup> — <sup>1</sup>Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany — <sup>2</sup>Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany — <sup>3</sup>Institute for the Dynamics of Complex Systems, University of Göttingen, 37077 Göttingen, Germany

As society paves its way towards devices miniaturization and precision medicine, micro-scale actuation and guided transport become increasingly prominent research fields, with high potential impact in both technological and clinical contexts. To accomplish directed motion of micron-sized cargos towards specific target sites, a promising strategy is the usage of living cells as smart biochemically-powered carriers, developing so-called bio-hybrid systems. In this talk, we discuss eukaryotic active particle transport, using *Dictyostelium discoideum* as a model organism. We shed light on the underlying mechanics and the emerging dynamics governing such cell-mediated transport. A simple yet powerful model is proposed which reproduces the observed phenomenology and, moreover, elucidates the role of cell-cargo interactions for the long-time mass transport efficiency.

CPP 11.3 Tue 11:40 DYa

**Predictive local field theories for interacting active Brownian spheres\*** — JENS BICKMANN and ●RAPHAEL WITTKOWSKI — Insti-

tut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

We present predictive local field theories for the dynamics of interacting spherical active Brownian particles in two and three spatial dimensions. Alongside the general theories, which include configurational order parameters and derivatives up to infinite order, we present reduced models that are easier to apply. We show that our theories contain popular models such as Active Model B + as special cases and that they provide explicit expressions for the coefficients occurring in these models. As further outcomes, the theories yield analytical expressions, e.g., for the density-dependent mean swimming speed and the spinodal corresponding to motility-induced phase separation of the particles. The analytical predictions are found to be in very good agreement with results of Brownian dynamics simulations and results from the literature.

\*Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1

CPP 11.4 Tue 12:00 DYa

**Dynamical States in Underdamped Active Matter with Anti-alignment Interaction** — ●DOMINIC AROLD<sup>1</sup> and MICHAEL SCHMIEDEBERG<sup>2</sup> — <sup>1</sup>TransDeNLab, UKD, Dresden, Germany — <sup>2</sup>Institut für Theoretische Physik 1, FAU, Erlangen, Germany

Many active matter systems, especially on the microscopic scale, are well approximated as overdamped, meaning that any inertial momentum is immediately dissipated by the environment. On the other hand, for macroscopic active systems, the time scale of inertial motion can become large enough to be relevant for the dynamics already on the single-particle level [1]. This raises the question of how collective dynamics and the resulting states in active matter are influenced by inertia. We propose a coarse-grained continuum model for underdamped active matter based on a dynamical density functional theory for passive systems [2]. Further, we apply the model to a system with short-range alignment and distant anti-alignment interaction known from the context of pattern formation. Our simulations of under- and overdamped dynamics both predict a structured laning state. However, activity-induced convective flows only present in the underdamped model destabilize this state when the anti-alignment is weakened, leading to a collective motion state which is not predicted in the overdamped limit. A turbulent transition regime between the two states is distinguished by strong density fluctuations and the absence of global ordering.

[1] Scholz C *et al.* 2018 *Nature communications* **9** 5156

[2] Archer A J 2009 *The Journal of chemical physics* **130** 014509

CPP 11.5 Tue 12:20 DYa

**Chemokinesis causes trapping and avoidance by dynamic**

**scattering** — ●JUSTUS KROMER<sup>1</sup> and BENJAMIN FRIEDRICH<sup>2,3</sup> — <sup>1</sup>Stanford University, Stanford, United States of America — <sup>2</sup>cfaed TU Dresden, Dresden, Germany — <sup>3</sup>PoL TU Dresden, Dresden, Germany

A minimal control strategy for artificial microswimmers with limited information processing capabilities is chemokinesis: the regulation of random directional fluctuations or speed as function of local, non-directional cues. In contrast to chemotaxis, it is not well understood whether chemokinesis is beneficial for the search for hidden targets.

We present a general theory of chemokinetic search agents that regulate directional fluctuations according to distance to a target. We characterize a dynamic scattering effect that reduces the probability to penetrate regions with strong directional fluctuations. If the target is surrounded by such a region, dynamic scattering causes beneficial inward-scattering of agents that had just missed the target, but also disadvantageous outward-scattering of agents approaching the target for the first time. If agents respond instantaneously to positional cues, outward-scattering dominates and chemokinetic agents perform worse than simple ballistic search. Yet, agents with just two internal states can decouple both effects and increase the probability to find the target significantly. We apply our analytical theory to the biological example of sperm chemotaxis of marine invertebrates. Sperm cells need to pass a 'noise zone' surrounding the egg, where chemokinesis masks chemotaxis. Kromer et al., PRL 124, 118101 (2020)

CPP 11.6 Tue 12:40 DYa

**Magnetic microswimmers exhibit Bose-Einstein-like condensation** — FANLONG MENG<sup>1</sup>, DAIKI MATSUNAGA<sup>2</sup>, ●BENOÎT MAHAULT<sup>3</sup>, and RAMIN GOLESTANIAN<sup>3</sup> — <sup>1</sup>CAS Key Laboratory for Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences — <sup>2</sup>Graduate School of Engineering Science, Osaka University — <sup>3</sup>Max Planck Institute for Dynamics and Self-Organization

We study an active matter system comprised of magnetic microswimmers confined in a microfluidic channel and show that it exhibits a new type of self-organized behavior. Combining analytical techniques and Brownian dynamics simulations, we demonstrate how the interplay of non-equilibrium activity, external driving, and magnetic interactions leads to the condensation of swimmers at the center of the channel via a non-equilibrium phase transition that is formally akin to Bose-Einstein condensation. We find that the effective dynamics of the microswimmers can be mapped onto a diffusivity-edge problem, and use the mapping to build a generalized thermodynamic framework, which is verified by a parameter-free comparison with our simulations. Our work reveals how driven active matter has the potential to generate exotic classical non-equilibrium phases of matter with traits that are analogous to those observed in quantum systems.

## CPP 12: Focus Phase Separation in Biological Systems II (joint session BP/CPP)

Time: Tuesday 14:00–16:00

Location: BPb

CPP 12.1 Tue 14:00 BPb

**Phase separation provides a mechanism to reduce noise in cells** — ●FLORIAN OLTSCH<sup>1,2</sup>, ADAM KLOSIN<sup>1</sup>, TYLER HARMON<sup>1,3</sup>, ALF HONIGMANN<sup>1,4</sup>, FRANK JÜLICHER<sup>2,3,4</sup>, ANTHONY HYMAN<sup>1,2,4</sup>, and CHRISTOPH ZECHNER<sup>1,2,4</sup> — <sup>1</sup>Max Planck Institute of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — <sup>2</sup>Center for Systems Biology Dresden, 01307 Dresden, Germany — <sup>3</sup>Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — <sup>4</sup>Cluster of Excellence Physics of Life, TU Dresden, 01062 Dresden, Germany

Noise in gene expression can cause significant variability in protein concentration. How cells buffer variation in protein concentration is an important question in biology. In this talk, I will show that liquid-liquid phase separation provides an effective mechanism to reduce variability in protein concentration. First, I will introduce our theoretical framework that discusses phase separation in the presence of active protein production and turnover. This stochastic non-equilibrium model allows us to study how fluctuations in protein concentration are affected by phase separation. I will then present under which physical conditions noise buffering by phase separation can be effective. Subsequently, I will show experimental data to test our theoretical predictions.

CPP 12.2 Tue 14:20 BPb

**Parasitic Behavior in Competing Dissipative Reaction Cycles** — ●PATRICK SCHWARZ<sup>1</sup>, SUDARSHANA LAHA<sup>3,4</sup>, JACQUELINE JANSSEN<sup>3,4</sup>, TABEA HUSS<sup>1</sup>, CHRISTOPH A. WEBER<sup>3,4</sup>, and JOB BOEKHOVEN<sup>1,2</sup> — <sup>1</sup>Department of Chemistry, Technische Universität München, Lichtenbergstrasse 4, 85748 Garching, Germany — <sup>2</sup>Institute for Advanced Study, Technische Universität München, Lichtenbergstrasse 2a, 85748 Garching, Germany — <sup>3</sup>Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — <sup>4</sup>Center for Systems Biology Dresden, CSBD, Dresden, Germany

Fuel-driven reaction cycles serve as model systems of the intricate reaction network of life. Rich and dynamic behavior is observed when such reaction cycles regulate phase separation or assembly. However, it remains unclear how the interplay between multiple reaction cycles affects their fate. To tackle this question, we created a library of precursor molecules that compete for a common fuel to transiently activate products. Generally, the competition for fuel means that a competitor decreases the success of the cycle. However, in cases where the transient competitor product can phase separate, this relation can be inverted. The presence of assemblies formed by such a competitor can increase the survival time of one product, analogous to how the

presence of a host can increase the survival time of a parasite. Our study of such a parasitic behavior in multiple fuel-driven reaction cycles represents a lifelike trait, paving the way for bottom-up design of synthetic life.

CPP 12.3 Tue 14:50 BPb

**Surface condensation of a pioneer transcription factor on DNA** — ●JOSE A. MORIN<sup>1,2</sup>, SINA WITTMANN<sup>1</sup>, SANDEEP CHOUBEY<sup>1,3</sup>, ADAM KLOSIN<sup>1</sup>, STEFAN GOLPIER<sup>1,3</sup>, ANTHONY A. HYMAN<sup>1,5</sup>, FRANK JÜLICHER<sup>3,4,5</sup>, and STEPHAN W. GRILL<sup>1,2,5</sup> — <sup>1</sup>Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany. — <sup>2</sup>Biotechnologisches Zentrum, Technische Universität Dresden, Dresden, Germany. — <sup>3</sup>Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — <sup>4</sup>Center for Systems Biology Dresden, Dresden, Germany. — <sup>5</sup>Cluster of Excellence Physics of Life, Technische Universität Dresden, Dresden, Germany.

Transcription factors cluster into sub-micrometer sized condensates while initiating transcription of their target genes. How cells achieve liquid-like clusters of constrained size at specific locations on DNA is not known. Here we investigate the role of DNA in the nucleation of condensates, using the pioneer transcription factor KLF-4. We show that KLF-4 forms liquid-like condensates on the DNA surface at physiological concentrations, below the one required for Klf4 phase separation. Through a dialogue between theory and experiments, we demonstrate that condensation occurs via a switch-like transition from a thin adsorbed layer to a thick condensed layer on DNA that is well described as a prewetting transition on a heterogeneous substrate. This phenomenon is thus a form of surface condensation mediated by and limited to the DNA surface.

## CPP 13: Complex Fluids and Soft Matter 3 (joint session DY/CPP)

Time: Tuesday 14:30–16:30

Location: DYc

CPP 13.1 Tue 14:30 DYc

**How Frost Forms and Grows on Lubricant Impregnated Surfaces** — ●LUKAS HAUER<sup>1</sup>, WILLIAM S.Y. WONG<sup>1</sup>, LOU KONDIC<sup>2</sup>, and DORIS VOLLMER<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>Department of Mathematical Sciences, NJIT, Newark, USA

In many technical applications the formation of frost and ice displays a hazard to the steady functionality of devices. This motivates the development of new materials to tackle the reduction of frosting and icing on surfaces. While icing on surfaces is commonly studied by localized nucleation mechanisms, the formation of frost is comparable more complicated: Formation of condensate droplets, freezing, and frost front propagation are multi-physical processes on multiple time and length scales. Lubricant impregnated surfaces are known for improved anti-icing properties. They experience lower ice drop adhesion and allegedly delayed surface frost formation. We show that frost formation can induce immensely strong capillary forces that could result in surface damage, lubricant depletion and the loss of anti-icing properties. Laser scanning confocal microscopy enables us to monitor the dynamic lubricant migration during condensation frosting on microstructured surfaces. We present a quantitative model of the lubricant migration, utilizing lubrication theory. This work serves to improve understanding of lubricant dynamics during condensation frosting, providing roadmaps towards the future design of anti-icing surfaces.

CPP 13.2 Tue 14:50 DYc

**Hydraulic and electric control of cell spheroids** — ●CHARLIE DUCLUT<sup>1</sup>, JACQUES PROST<sup>2</sup>, and FRANK JÜLICHER<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — <sup>2</sup>Laboratoire Physico Chimie Curie, Institut Curie, Paris, France — <sup>3</sup>Center for Systems Biology Dresden, Germany

In addition to generating forces and reacting to mechanical cues, tissues are capable to actively pump fluid and create electric current. In this talk, we will discuss how a hydraulic or electrical perturbation, imposed for instance by a drain of micrometric diameter, can be used to perturb tissue growth dynamics. We address this issue in a continuum description of a spherical cell assembly that includes the mechanical, electrical and hydraulic properties of the tissue. This approach allows us to discuss and quantify the effect of electrohydraulic perturbations on the long-time states of the tissue. We highlight that a

CPP 12.4 Tue 15:10 BPb

**Slowing down protein aggregation in liquid compartments** — ●WOJCIECH P. LIPIŃSKI<sup>1</sup>, BRENT VISSER<sup>1</sup>, MIREILLE CLAESSENS<sup>2</sup>, MOHAMMAD A. A. FAKHREE<sup>2</sup>, SASKIA LINDHOUD<sup>3</sup>, and EVAN SPRUIJT<sup>1</sup> — <sup>1</sup>Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — <sup>2</sup>Nanobiophysics, Faculty of Science and Technology, University of Twente, Enschede, the Netherlands — <sup>3</sup>Molecular Nanofabrication, Faculty of Science and Technology, University of Twente, Enschede, the Netherlands

With increasing life expectancy in modern societies, amyloid-related diseases are becoming alarmingly common. Extensive work has been done to investigate the kinetics of amyloid formation and the structure of aggregates. Recently it has been suggested that protein aggregation can be influenced by the presence of membraneless organelles. Aggregation-prone proteins may be sequestered by liquid compartments, leading to significant changes in concentration and altered aggregation kinetics.

Here, we present a combined computational and experimental study of the fate of aggregation-prone proteins that are sequestered by liquid droplets. We investigated computationally the influence of varying parameters describing aggregation and transport processes and showed that aggregation process can be either accelerated or inhibited by the presence of liquid compartments. Motivated by these findings we have undertaken efforts to develop experimental systems exhibiting diversified influence of the phase-separated environment on the protein aggregation process.

30 min. Meet the Speaker

sufficiently strong external flow or electric current can drive a proliferating spheroid to decay. We propose that this could have applications in medicine.

CPP 13.3 Tue 15:10 DYc

**Controlling Elastic Turbulence** — ●REINIER VAN BUEL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Controlling the flow patterns of viscoelastic fluids is extremely challenging due to their inherent non-linear and time-dependent properties. These complex fluids exhibit transitions from laminar to turbulent flows, which is useful for heat and mass transport in liquids at the micron scale [1], whereas in Newtonian fluids transport is dominated by diffusion. Turbulent viscoelastic flows show similar properties as their counterparts in Newtonian fluids [1,2] and consequently the observed flow pattern is called *elastic turbulence* [1]. It occurs in shear flow for increasing Weissenberg number  $Wi$ , the product of polymer relaxation time and shear rate.

Numerically solving the Oldroyd-B model in a two-dimensional Taylor-Couette geometry, we have identified and described the supercritical transition to turbulent flow at a critical Weissenberg number [2]. Here, we demonstrate that elastic turbulence can be controlled by a time-modulated shear rate. The order parameter measuring the strength of turbulence continuously goes to zero with increasing modulation frequency or Deborah number  $De$ . It ultimately vanishes via a supercritical transition, where flow then becomes laminar. Moving closer to the critical Weissenberg number, smaller modulation frequencies are sufficient to induce laminar flow.

[1] A. Groisman and V. Steinberg, *Nature* **405**, 53 (2000).

[2] R. Buel, C. Schaaf, H. Stark, *Europhys. Lett.* **124**, 14001 (2018).

CPP 13.4 Tue 15:30 DYc

**Hydrodynamics of a Pair of Soft Capsules in Inertial Microfluidics** — ●KUNTAL PATEL and HOLGER STARK — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

In recent years, inertial microfluidics has emerged as a robust technique to precisely manipulate solid particles and biological cells. Also, the fact that inertial microfluidics operates at finite Reynolds numbers enables to achieve high throughput. In the present work, we perform 3D numerical simulations to study the hydrodynamic interaction and inertial migration of two soft capsules in a microchannel with quadratic

cross section. We employ the lattice Boltzmann method to determine fluid flow and the finite element method to model capsule dynamics. The coupling between bulk fluid and capsules is realized using the immersed boundary method.

We investigate the effect of different starting positions for mono- and bi-dispersed pairs of varying softness and capsule shape. Based on the temporal evolution of interparticle distance, we characterize the dynamics of various mono- and bi-dispersed pairs into four types: stable pair, stable pair with damped oscillations, stable pair with bounded oscillations, and unstable pair. We observe that stable pairs become unstable when increasing the particle stiffness. Furthermore, a pair with both capsules in the same channel half is more prone to become unstable than a pair with capsules in the opposite channel halves.

CPP 13.5 Tue 15:50 DYc

#### Hydrodynamics of immiscible binary fluids with viscosity contrast: A Multiparticle Collision Dynamics approach

— •ZIHAN TAN<sup>1</sup>, VANIA CALANDRINI<sup>2</sup>, JAN DHONT<sup>1</sup>, GERHARD NÄGELE<sup>1</sup>, and ROLAND WINKLER<sup>3</sup> — <sup>1</sup>Biomacromolecular Systems and Processes, Institute of Biological Information Processing, Forschungszentrum Jülich, 52428 Jülich, Germany — <sup>2</sup>Computational Biomedicine, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany — <sup>3</sup>Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

By coupling distinct collision steps in each fluid domain, immiscible binary fluids with different viscosities connected by coarse-grained planar interfaces are realized by multiparticle collision dynamics (MPC). The flow and the stress-viscosity relation of the system are investigated under shear flow, excellently agree with continuum hydrodynamics solution and the analytical theory of MPC. Later, the hydrodynamic mobility coefficients of an embedded colloid close to the fluid-fluid interface are measured, which coincide with hydrodynamic multipole

expansion calculations. To validate the length and time scales of hydrodynamics in this model, we explore the corresponding transverse velocity correlations. It is found that the correlations for the fluid regions occupied by one phase are identical to single-phase MPC fluid. In contrast, the transverse modes at the interfacial region can be interpreted by the superposition of both viscous components.

CPP 13.6 Tue 16:10 DYc

#### Optimal hematocrit for ATP release by red blood cell in microcirculation — •ZHE GOU and CHAOQI MISBAH — Laboratoire Interdisciplinaire de Physique, Grenoble, France

ATP release by red blood cells (RBCs) acts as an important signaling molecule for various physiological functions, such as vasodilation. When flowing in microcirculation, RBCs experience a cascade of branching vessels, from arterioles to capillaries, and finally to venules, which affects not just flow behavior of blood but also ATP release. In a previous study, we have proposed a model of ATP release by RBCs through two pathways of cell membrane: pannexin 1 channel (Px1), sensitive to shear stress, and cystic fibrosis transmembrane conductance regulator (CFTR) which responds to cell deformation. As a continuation, present work further investigates the effect of flow strength, hematocrit, and vascular diameter by numerical simulations. We found a nontrivial spatial RBC organization and ATP patterns due to application of shear stress on the RBC suspension. Conditions for optimal ATP release per cell are identified, which depend on vessel size and hematocrit Ht. Increasing further Ht beyond optimum enhances the total ATP release but should degrade oxygen transport capacity, a compromise between an efficient ATP release and minimal blood dissipation. Moreover, ATP is boosted in capillaries suggesting a vasomotor activity coordination throughout the resistance network. Further studies of vascular network may help to explore the whole signaling cascade of ATP.

## 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<sup>1,2</sup>, ANGEL ALEGRÍA<sup>1,3</sup>, JÜRGEN ALLGEIER<sup>4</sup>, MARGARITA KRUTEVA<sup>4</sup>, INGO HOFFMANN<sup>5</sup>, SYLVAIN PRÉVOST<sup>5</sup>, MICHAEL MONKENBUSCH<sup>4</sup>, DIETER RICHTER<sup>4</sup>, ARANTXA ARBE<sup>1</sup>, and JUAN COLMENERO<sup>1,3,6</sup> — <sup>1</sup>Materials Physics Center (CSIC-UPV/EHU), San Sebastian, Spain — <sup>2</sup>IKERBASQUE - Basque Foundation for Science, Bilbao, Spain — <sup>3</sup>Departamento de Física de Materiales (UPV/EHU), San Sebastian, Spain — <sup>4</sup>Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>5</sup>Institut Laue-Langevin, Grenoble, France — <sup>6</sup>Donostia 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 CAO<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, ANDREI CHUMAKOV<sup>2</sup>, MATTHIAS OPEL<sup>3</sup>, MARKUS GALLET<sup>4</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2,5</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,6</sup> — <sup>1</sup>TU München, Physik-Department, 85748 Garching — <sup>2</sup>DESY, 22607 Hamburg — <sup>3</sup>WMI, Bayerische Akademie der Wissenschaften, 85748 Garching — <sup>4</sup>Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — <sup>5</sup>KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 44 Stockholm, Sweden

— <sup>6</sup>TU 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 EVERETT<sup>1</sup>, MARTINA PLANK<sup>2</sup>, MARKUS GALLET<sup>3</sup>, MATTHIAS SCHWARTZKOPF<sup>4</sup>, STEPHAN ROTH<sup>4,5</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,6</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — <sup>2</sup>TU Darmstadt, Ernst-Berl-Institute, Darmstadt, Germany — <sup>3</sup>Saarland University, Chair in Polymer Chemistry, Saarbrücken, Germany — <sup>4</sup>Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — <sup>5</sup>KTH Royal Institute of Technology, Stockholm, Sweden — <sup>6</sup>Heinz 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 (Fe<sub>3</sub>O<sub>4</sub>) nanoparticles (NPs). Through solvent vapor annealing, nanostruc-

tured 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 LI<sup>1</sup>, CHIA-HSIN KO<sup>1</sup>, ATHANASIOS SKANDALIS<sup>2</sup>, DMITRY MOLODENSKIY<sup>3</sup>, STERGIOS PISPAS<sup>2</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, Physik weicher Materie, Garching, Germany — <sup>2</sup>Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — <sup>3</sup>EMBL 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 YIN<sup>1</sup>, WEI CAO<sup>1</sup>, QING JI<sup>2</sup>, YAJUN CHENG<sup>2</sup>, LIN SONG<sup>3</sup>, NIAN LI<sup>1</sup>, CHRISTIAN L. WEINDL<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>4</sup>, STEPHAN V. ROTH<sup>4,5</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,6</sup> — <sup>1</sup>Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — <sup>2</sup>Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, Ningbo, 315201, P. R. China — <sup>3</sup>Northwestern Polytechnical University, Xi'an 710072, China. — <sup>4</sup>DESY, Notkestr. 85, 22603 Hamburg, Germany — <sup>5</sup>Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — <sup>6</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

We systematically investigate the synthesis of polystyrene-block-poly(4-vinylpyridine) templated Fe<sub>2</sub>O<sub>3</sub> thin films by changing the solvent category (DMF or 1,4-dioxane) and the polymer-to-FeCl<sub>3</sub> 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<sup>1,2</sup>, MARIE BETKER<sup>1,3</sup>, ALEXANDROS ALEXAKIS<sup>3</sup>, ANDREI CHUMAKOV<sup>1</sup>, ELISABETH ERBES<sup>1,4</sup>, MARC GENSCH<sup>1,2</sup>, QING CHEN<sup>1</sup>, JAN RUBECK<sup>1</sup>, NILS LE COUTRE<sup>5</sup>, CALVIN J. BRETT<sup>1,3</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, EVA MALMSTRÖM<sup>3</sup>, DANIEL SÖDERBERG<sup>3</sup>, PETER MÜLLER-BUSCHBAUM<sup>2</sup>, and STEPHAN V. ROTH<sup>1,3</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany — <sup>2</sup>Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — <sup>3</sup>KTH Royal Institute of Technology, Teknikringen 56-58, SE-100 44 Stockholm, Sweden — <sup>4</sup>Institute for X-ray Physics, Goettingen University, Friedrich Hund Platz 1, 37077 Goettingen, Germany — <sup>5</sup>Universität Rostock, Universitätsplatz 1, 18055 Rostock, Germany

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  $\beta$ -lactoglobulin in biotemplating TiO<sub>2</sub> during spray deposition with in situ GIXS techniques: A route to green sol-gel chemistry** — ●JULIAN E. HEGER<sup>1</sup>, WEI CHEN<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, CHRISTIAN L. WEINDL<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, CALVIN J. BRETT<sup>2,3</sup>, WIEBKE OHM<sup>3</sup>, STEPHAN V. ROTH<sup>2,3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — <sup>2</sup>Royal Institute of Technology KTH, Teknikringen 34-35, 100 44 Stockholm, Sweden — <sup>3</sup>Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — <sup>4</sup>Heinz 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  $\beta$ -lactoglobulin ( $\beta$ -lg), which is known to form different aggregates as a function of net charge controlled by pH during denaturation. For this,  $\beta$ -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 (GIXS) synchrotron techniques identify the underlying kinetics of  $\beta$ -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 YAZDANSHENAS<sup>1</sup>, BART-JAN NIEBUUR<sup>1</sup>, DIRK SCHANZENBACH<sup>2</sup>, ANDRÉ LASCHEWSKY<sup>2,3</sup>, MICHAELA ZAMPONI<sup>4</sup>, DARIA NOFERINI<sup>4</sup>, ALFONS SCHULTE<sup>5</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, Garching — <sup>2</sup>Universität Potsdam, Institut für Chemie — <sup>3</sup>Fraunhofer IAP, Potsdam-Golm — <sup>4</sup>FZ Jülich, JCNS at MLZ, Garching — <sup>5</sup>University 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 H<sub>2</sub>O, 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-PNIPAM films** — ●JULIJA REITENBACH<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, GAETANO MANGIAPIA<sup>2</sup>, CRISTIANE HENSCHL<sup>3</sup>, ANDRÉ LASCHEWSKY<sup>3</sup>, CHRISTINE PAPADAKIS<sup>4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching — <sup>2</sup>Helmholtz-Zentrum Geesthacht am Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85748 Garching — <sup>3</sup>Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm — <sup>4</sup>TU München, Physik-Department, Physik weicher Materie, James-Franck-Str. 1, 85748 Garching

Thin films of the thermoresponsive diblock copolymer PMMA-b-PNIPAM 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 WIDMANN<sup>1</sup>, LUCAS P. KREUZER<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, JULIAN E. HEGER<sup>1</sup>, GAETANO MANGIPIA<sup>2</sup>, THOMAS HELLWEG<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>HZG at MLZ, 85748 Garching — <sup>3</sup>Universität 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 ZALUZHNYI<sup>1</sup>, RUSLAN KURTA<sup>2</sup>, MARCUS SCHEELE<sup>3</sup>, FRANK SCHREIBER<sup>1</sup>, BORIS OSTROVSKII<sup>4</sup>, and IVAN VARTANYANTS<sup>5,6</sup> — <sup>1</sup>Institute of Applied Physics, University of Tübingen, Tübingen, Germany — <sup>2</sup>European XFEL, Schenefeld, Germany — <sup>3</sup>Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany — <sup>4</sup>Federal Scientific Research Center "Crystallography and photonics", Moscow, Russia — <sup>5</sup>Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — <sup>6</sup>National 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 supracolloidal magnetic polymers in microchannel under external field** — •VLADIMIR ZVEREV<sup>1</sup>, EKATERINA NOVAK<sup>1</sup>, SOFIA KANTOROVICH<sup>2,1</sup>, and PEDRO SÁNCHEZ<sup>2,1</sup> — <sup>1</sup>Ural Federal University, Ekaterinburg, Russia — <sup>2</sup>University of Vienna, Vienna, Austria

Advances in synthesis technology in the field of magnetoreactive polymer 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 NOVAK<sup>1</sup>, VLADIMIR ZVEREV<sup>1</sup>, MARINA GUPALO<sup>1</sup>, and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>Ural Federal University, Ekaterinburg, Russia — <sup>2</sup>University 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. WEINDL<sup>1</sup>, CHRISTIAN FAJMAN<sup>2</sup>, MICHAEL A. GIEBEL<sup>2</sup>, MATTHIAS SCHWARZKOPF<sup>3</sup>, STEPHAN V. ROTH<sup>3,4</sup>, THOMAS F. FÄSSLER<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>Technische Universität München, Physik Department, Lehrstuhl für Funktionelle Materialien, James-Frankstraße 1, 85748 Garching, Germany — <sup>2</sup>Technische Universität München, Chemie-Department, Lehrstuhl für anorganische Chemie mit Schwerpunkt Neue Materialien, Lichtenbergstr. 4, 85748 Garching, Germany — <sup>3</sup>Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — <sup>4</sup>Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — <sup>5</sup>Heinz 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 REB<sup>1</sup>, MICHAEL BÖHMER<sup>2</sup>, BENJAMIN PREDESCHLY<sup>1</sup>, SEBASTIAN GROTT<sup>1</sup>, CHRISTIAN WEINDL<sup>1</sup>, GORAN IVANDEKIC<sup>1</sup>, RENJUN GUO<sup>1</sup>, CHRISTOPH DREISSIGACKER<sup>3</sup>, ROMAN GERNHÄUSER<sup>2</sup>, ANDREAS MEYER<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — <sup>2</sup>TU München, Physik-Department, Zentrales Technologielabor, Garching, Germany — <sup>3</sup>Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, Germany — <sup>4</sup>Heinz Maier-Leibnitz-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<sup>-2</sup>, whereas both bulk heterojunction absorber PBDB-T:ITIC and PTB7-Th:PC71BM organic solar cell types reached more than 4 and 7 mW cm<sup>-2</sup>, 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 LI<sup>1</sup>, RENJUN GUO<sup>1</sup>, WEI CHEN<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, JULIAN E. HEGER<sup>1</sup>, SUZHE LIANG<sup>1</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — <sup>2</sup>Deutsches 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 TiO<sub>2</sub>/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*<sub>sc</sub>) 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 GUO<sup>1</sup>, DAN HAN<sup>2</sup>, WEI CHEN<sup>1</sup>, LINJIE DAI<sup>3</sup>, KANGYU JI<sup>3</sup>, QIU XIONG<sup>4</sup>, SAISAI LI<sup>5</sup>, LENNART K. REB<sup>1</sup>, MANUEL A. SCHEEL<sup>1</sup>, SHAMBHAVI PRATAP<sup>1</sup>, NIAN LI<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, TIANXIAO XIAO<sup>1</sup>, SUZHE LIANG<sup>1</sup>, ANNA-LENA OECHSLE<sup>1</sup>, CHRISTIAN L. WEINDL<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>6</sup>, HUBERT EBERT<sup>2</sup>, PENG GAO<sup>4</sup>, MINGJIAN YUAN<sup>5</sup>, NEIL C. GREENHAM<sup>3</sup>, SAMUEL D. STRANKS<sup>3</sup>, STEPHAN V. ROTH<sup>6</sup>, RICHARD H. FRIEND<sup>3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München — <sup>2</sup>James-Franck-Str. 1 — <sup>3</sup>University of Cambridge — <sup>4</sup>Chinese Academy of Sciences — <sup>5</sup>Nankai University — <sup>6</sup>Deutsche 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 MAPbI<sub>3</sub>-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



**The Role of CsBr in Crystal Orientation and Optoelectronic Properties of MAPbI<sub>3</sub>-based devices** — •YUQIN ZOU and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Frank-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 14.23 Tue 16:30 CPPp

**Energetics of lead halide perovskite precursors in different solvents** — •RICHARD SCHIER<sup>1</sup>, ANA M. VALENCIA<sup>2</sup>, and CATERINA COCCHI<sup>2</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin — <sup>2</sup>Carl 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  $PbX_2M_4$ , 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 MAPbI<sub>3</sub> perovskite via dual frequency resonance tracking PFM** — •ILKA HERMES<sup>1</sup> and RO-MAIN STOMP<sup>2</sup> — <sup>1</sup>Park Systems Europe, Mannheim, Germany — <sup>2</sup>Zuerich Instruments, Zuerich, Switzerland

Methylammonium lead iodide (MAPbI<sub>3</sub>)-based photovoltaics have seen an astonishing increase in efficiency due to their unique optoelectronic properties and charge carrier dynamics. Since MAPbI<sub>3</sub> 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 MAPbI<sub>3</sub> 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 MAPbI<sub>3</sub> domains.

CPP 14.25 Tue 16:30 CPPp

**In situ phase and texture evolution tracking of the formation of 2-step slot-die coated perovskite by GIWAXS** — •MANUEL A. SCHEEL<sup>1</sup>, LENNART K. REB<sup>1</sup>, RENJUN GUO<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, STEPHAN V. ROTH<sup>2,3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>Lehrstuhl für Funktionelle Materialien, Physik-Department — <sup>2</sup>DESY, Notkestr. 85, 22607 Hamburg — <sup>3</sup>KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — <sup>4</sup>Heinz 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 PbI<sub>2</sub>, MAI and MAPbI<sub>3</sub> 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 PROCIDA<sup>1</sup>, RICHARD SCHIER<sup>2</sup>, ANA VALENCIA<sup>1,2</sup>, and CATERINA COCCHI<sup>1,2</sup> — <sup>1</sup>Institut für Physik, Carl von Ossietzky Universität Oldenburg — <sup>2</sup>Institut 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  $PbX_2(Sol)_4$  compounds in solution, where  $X=Cl, Br, I$ , 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.

## CPP 15: Nationale Forschungsdateninfrastruktur (NDFI) (joint session BP/CPP/DY/SOE)

Time: Tuesday 17:45–18:30

Location: BPb

Details will be published in a programme update.

## CPP 16: Charged Soft Matter - organized by Joachim Dzubiella (Albert Ludwigs University Freiburg, Freiburg)

Time: Wednesday 9:00–15:20

Location: CPPa

### Invited Talk

CPP 16.1 Wed 9:00 CPPa  
**Charging Dynamics and Structure of Ionic Liquids in Nanoporous Supercapacitors** — ●CHRISTIAN HOLM<sup>1</sup>, KONRAD BREITSPRECHER<sup>1</sup>, and SVYATOSLAV KONDRAT<sup>2,3</sup> — <sup>1</sup>University of Stuttgart, Institute for Computational Physics, Stuttgart, Germany — <sup>2</sup>Department of Complex Systems, Polish Academy of Sciences, Warsaw, Poland — <sup>3</sup>MPI for Intelligent Systems, Stuttgart, Germany

Ionic liquid based nanoporous supercapacitors have recently attracted much attention as energy storage devices with remarkable cyclability and high power and energy densities. However, their use in high-frequency applications might be limited by a relatively slow charging process. In this talk we will first discuss the fluid structure within a slit-pore capacitor system [1] and report on the physics and optimization of charge/discharge cycles [2,3]. We will see that step-voltage charging is slow because the coions become trapped in narrow pores of the supercapacitor electrodes. To avoid such trapping, a slow voltage-sweep charging is considered, which allows to accelerate the overall charging process substantially. We furthermore examine in detail the discharging process, as well. At the end we will report on the effect of nonlinear charging functions.

[1] K. Breitsprecher, M. Abele, S. Kondrat and C. Holm, *J. Chem. Phys.*, 147, 104708 (2017).

[2] K. Breitsprecher, C. Holm, S. Kondrat, *ACS nano* 12 (10), 9733-9741 (2018) .

[3] K. Breitsprecher et al., *Nature Communications* 11, 6085 (2020)

CPP 16.2 Wed 9:40 CPPa

**Structure and Relaxation Dynamics of an Ionic Liquid in Molecular Scale Confinement.** — ●MARKUS MEZGER<sup>1</sup>, HENNING WEISS<sup>1</sup>, JULIAN MARS<sup>1</sup>, HSIU-WEI CHENG<sup>2</sup>, MARKUS VALTNER<sup>2</sup>, and VEIJO HONKIMAEKI<sup>3</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>TU Wien, Institute for Applied Physics, Vienna, Austria — <sup>3</sup>ESRF-The European Synchrotron, Grenoble, France

Structure and dynamics of a confined ionic liquids were probed by an in-situ X-ray surface force apparatus in plane-cylinder geometry. Our novel device can shear, compress and decompress soft matter within a precisely controlled slit pore confinement. Complementary structural information is obtained by X-ray scattering and simultaneous force measurements. Here, we present results from the wet ionic liquid C<sub>10</sub>mim<sup>+</sup>Cl<sup>-</sup> in its columnar liquid crystalline mesophase. Defect-formation and structural relaxation processes in confinement were studied as reaction to external stimuli. The observed mesoscopic orientation induced by oscillatory shear is explained by the anisotropic mobility of the amphiphilic cations.

Reference: H. Weiss et al., *Structure and Dynamics of Confined Liquids - Challenges and Perspectives for the X-Ray Surface Force Apparatus*. *Langmuir*, DOI: 10.1021/acs.langmuir.9b01215 (2019).

CPP 16.3 Wed 10:00 CPPa

**Hydrogen Bonding and Charge Transport in a Protic Polymerized Ionic Liquid** — ●ARTHUR MARKUS ANTON<sup>1,2</sup>, FALK FRENZEL<sup>2</sup>, JIAYIN YUAN<sup>3</sup>, MARTIN TRESS<sup>2,4</sup>, and FRIEDRICH KREMER<sup>2</sup> — <sup>1</sup>The University of Sheffield, Department for Physics & Astronomy, Sheffield, UK — <sup>2</sup>Leipzig University, Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — <sup>3</sup>Stockholm University, Department of Materials and Environmental Chemistry, Stockholm, Sweden — <sup>4</sup>University of Tennessee Knoxville, Department of Chemistry, Knoxville, USA

Fourier transform infrared and broadband dielectric spectroscopy are combined in order to study hydrogen bonding and charge transport in the protic polymerized ionic liquid PAAPS in a wide temperature range from 170 to 300K. While the former allows to follow the formation of hydrogen bonds, the latter enables to record the complex conductivity in the spectral range from 10<sup>-2</sup> to 10<sup>+9</sup> Hz. On the one hand, the formation of the H-bond network exhibits a pronounced thermal hysteresis, whereas, on the other hand, the effective conductivity is reversibly affected by temperature. In combination with the fact that the conductivity changes with temperature by orders of magnitude, whereas the integrated absorbance of the N-H stretching vibration (being proportional to the number density of protons in the

hydrogen bond network) changes only by a factor of 4, it is concluded that charge transport takes place predominantly due to dynamic glass transition assisted hopping conduction mechanism and is not significantly affected by the establishment of H-bonds.

### 40 min. meet the speakers - break

### Invited Talk

CPP 16.4 Wed 11:00 CPPa  
**Interaction of polyelectrolytes with proteins** — ●MATTHIAS BALLAUFF — Institut für Chemie und Biochemie, Freie Universität Berlin

Highly charged natural polyelectrolytes as e.g. DNA or heparin play a central role in many biochemical processes and their interaction with proteins is of central importance as shown in a recent review [1]. In this lecture I shall review our studies of the interaction of well-defined synthetic polyelectrolytes with proteins that have been done mainly by calorimetry. There are two main factors that lead to the formation of a complex between a protein and a polyelectrolyte: i) The release of counterions condensed onto the highly charged polyelectrolyte, and ii) The release or uptake of water during complex formation. Systematic studies of the binding constant  $K_b$  as the function of temperature and salt concentration allow us to determine the contributions of both effects to the measured free energy of binding. This can be demonstrated by analyzing the binding of model proteins as lysozyme to well-characterized polyelectrolytes as e.g. heparin. The improved understanding of this complex formation may have direct medical implications as e.g. for virus binding to cell surfaces.

[1] K. Achazi, et al., *Understanding the Interaction of Polyelectrolyte Architectures with Proteins and Biosystems*, *Angew. Chem. Int. Ed.* 2020, 59, 2-25

CPP 16.5 Wed 11:40 CPPa

**Identifying Mg<sup>2+</sup> binding sites on RNA using MD simulations with accelerating force field parameters** — ●KARA K. GROTZ, SERGIO CRUZ-LEÓN, and NADINE SCHWIERZ — Department of Theoretical Biophysics, Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Mg<sup>2+</sup> is one of the most abundant cations in living cells. The interaction between Mg<sup>2+</sup> and RNA is essential for folding and function of the diverse macromolecule. Mg<sup>2+</sup> binds specifically and often directly (inner-sphere configuration) to individual functional groups on the RNA. Localizing Mg<sup>2+</sup> binding sites, however, is challenging as Mg<sup>2+</sup> is silent in most experimental approaches. Computational studies can contribute molecular insight but often struggle with insufficiently accurate atomistic models (force fields) and time scale limitations due to the slow binding kinetics of Mg<sup>2+</sup> (millisecond time scale). Herein, we use a recently developed Mg<sup>2+</sup> force field that is based on ion-water and ion-ion properties of Mg<sup>2+</sup>. In addition, the parameters are chosen such that they accelerate the water exchange kinetics (nanosecond time scale). Moreover, by incorporating experimental binding affinities towards specific RNA binding positions, we are able to find Mg<sup>2+</sup> binding sites on RNA using unbiased simulations and observe outer-to-inner sphere transitions directly.

CPP 16.6 Wed 12:00 CPPa

**Thermodynamics of Liquid-Liquid Phase Separation: Isothermal Titration Calorimetry of Hyaluronic Acid-Chitosan Coacervates** — FATMA AKCAY OGUR and ●A. BASAK KAYITMAZER — Department of Chemistry, Bogazici University Istanbul, Turkey

Complex coacervation occurs between two oppositely charged macromolecules which undergo into macroscopic phase separation and form two liquid phases: polyelectrolyte-rich (coacervate) and polyelectrolyte-poor (dilute) liquid phases. Coacervation has several application areas including processed food, cosmetics, paper, textiles, pharmaceutical and food industries. For these industrial applications, coacervation is utilized as a microencapsulation platform for drugs, aromas, odors, and flavors. Recently, liquid-liquid phase separation has been shown to be the driving force for membraneless organelles such as P granules and nucleoli. In our study, we have studied a model coacervate system composed of two oppositely charged polysaccha-

rides, i.e. namely, hyaluronic acid (HA) and chitosan (CH). Isothermal titration calorimetry (ITC) was employed to understand the thermodynamic characteristics of complex coacervation between these semiflexible biopolymers. Parameters (molecular weight of polyelectrolytes, pH and ionic strength of the medium, and temperature) that affect coacervation were studied to determine enthalpy change and binding constant of soluble complexes, stoichiometry of soluble complexes and coacervation, and molar heat capacity.

CPP 16.7 Wed 12:20 CPPa

**The effects of ethanol and salt on the phase behavior and interactions of aqueous protein solutions** — RAJEEVANN UTHAYAKUMAR, •FLORIAN PLATTEN, and STEFAN U. EGELHAAF — Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany

The addition of salts or organic solvents to aqueous protein solutions alters their optical and dielectric properties and the interactions between protein molecules in these mixtures change accordingly. Here, the effects of NaCl and ethanol on the phase behavior and interactions of protein solutions are studied in terms of the metastable liquid-liquid phase separation and second virial coefficient  $B_2$  of lysozyme solutions. The cloud-point temperatures are reduced and raised by the addition of ethanol and salt, respectively. The extended law of corresponding states allows to interpret these trends as changes of  $B_2$ . Remarkably, the dependence of  $B_2$  on both salt and ethanol content is quantitatively modelled by the DLVO theory.

CPP 16.8 Wed 12:40 CPPa

**Surface morphology of polyelectrolyte multilayer films with short PSS chains in water and air. Determining the surface elasticity of nanofilms** — •AMIR AZINFAR<sup>1</sup>, SVEN NEUBER<sup>1</sup>, JIŘÍ VANĚČEK<sup>2</sup>, MARIE VANCOVÁ<sup>2,3</sup>, JAN STERBA<sup>2,3</sup>, VÍTĚZSLAV STRAŇÁK<sup>3</sup>, and CHRISTIANE A. HELM<sup>1</sup> — <sup>1</sup>Institute of Physics - Angewandte Physik, University of Greifswald, Felix-Hausdorff-Str. 6, 17489 Greifswald, Germany — <sup>2</sup>Institute of Parasitology, Biology Centre, Czech Academy of Sciences, Branisovska 31, 37005 Ceske Budejovice, Czech Republic — <sup>3</sup>Faculty of Science, University of South Bohemia, Branisovska 1760, 37005 Ceske Budejovice, Czech Republic

We investigate the surface topology of polyelectrolyte multilayers made by sequential adsorption of polycations (PDADMA) and polyanions (low molecular weight PSS). We observed a buckling pattern of the film surface in air. The surface roughness  $\sigma$ (AFM) in air was always twice as high as in water. For PSS-terminated films, the periodicity of buckling patterns increased with the number of deposited layers from 185 nm to 225 nm. If the multilayer film was terminated with a PDADMA layer, the surface roughness  $\sigma$ (AFM) and the surface periodicity of buckling patterns were always bigger than for films terminated by a PSS layer. This is attributed to the larger surface coverage of PDADMA caused by its small linear charge density. We determined the surface elasticity of the film in non-linear and linear growth regimes by considering the surface strain and surface periodicity, and thus provide a model to explain the increase of periodicity with film thickness.

60 min. meet the speakers - break

CPP 16.9 Wed 14:00 CPPa

**Ion Correlations in Polymer Electrolyte-Ionic Liquid Mixtures** — •DIDDO DIDDENS<sup>1</sup> and ANDREAS HEUER<sup>1,2</sup> — <sup>1</sup>Helmholtz-Institut Münster (IEK-12), Forschungszentrum Jülich GmbH, Corrensstraße 46, 48149 Münster — <sup>2</sup>Institut für physikalische Chemie, Westfälische Wilhelms-Universität Münster, Corrensstraße 28/30, 48149 Münster

Polymer electrolytes consist of a salt dissolved in a polymer matrix such as poly(ethylene oxide) (PEO). Even though they are safer than conventional liquid battery electrolytes due to their reduced flammability and mechanical stability, their conductivity is still too low for an efficient technological use. To overcome this issue, the use of small molecular shuttles has been proposed [1], in which the cation of an ionic liquid (IL) is functionalized by a small oligoether side chain that can detach the lithium ions from the slow PEO chains. Additionally, dynamically coupling the lithium ions to the IL cations in this way, it is expected that IL and lithium cations move cooperatively in an electric field, giving rise to enhanced transference numbers. In this contribution, we explicitly check this assumption by focusing on dynamical ion correlations within the electrolyte, and on their impact on the lithium transference number as well as the overall conductivity.

[1] D. Diddens *et al.*, *J. Electrochem. Soc.* **2017**, 164, E3225

CPP 16.10 Wed 14:20 CPPa

**Local dynamics of ionic liquids studied by <sup>2</sup>H NMR** — •ELISA STEINRÜCKEN, MANUEL BECHER, and MICHAEL VOGEL — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

Room Temperature Ionic Liquids (RTIL) are molten salts at ambient temperatures with a low vapour pressure. They are usually glass forming systems with complex and heterogeneous molecular dynamics. The combination of different cations and anions opens wide ranges of chemical and physical applications. Hence, a fundamental understanding of molecular dynamics is of crucial importance. Here, RTILs consisting of imidazole-based cations and [TF<sub>2</sub>N]<sup>-</sup> or [BF<sub>4</sub>]<sup>-</sup> anions are in the experimental focus. Nuclear Magnetic Resonance (NMR) provides access to dynamics in wide ranges of time and length scales [M. Becher, E. Steinrücken, M. Vogel, *J. Chem. Phys.*, 2019]. Due to its isotope selectivity the dynamical behaviour of the two components can be distinguished. Performing <sup>2</sup>H NMR experiments on selectively deuterated cations, we gain deep insights into their microscopic rotational dynamics. When combining <sup>2</sup>H spin-lattice relaxation (SLR) and stimulated-echo (STE) experiments, rotational correlation times of the cation are accessible from the fast motion in the liquid to slow glassy dynamics. Furthermore, we exploit that STE experiments and <sup>2</sup>H line-shape analysis provide information about the mechanism for rotational motion. Altogether, we show that application of <sup>2</sup>H NMR to RTIL has a high potential for the characterization of time scales and motional mechanisms of the molecular dynamics.

CPP 16.11 Wed 14:40 CPPa

**Chain length dependent structure and dynamics of imidazolium based ionic liquids mixtures with water.** — •SEBASTIAN KLOTH and MICHAEL VOGEL — TU Darmstadt, Institut für Physik kondensierter Materie, Hochschulstr. 6, 64289, Darmstadt, Germany

With the huge amount of possible combinations, ionic liquids can be tailored to different properties and applications. In particular, the application as a "green" solvent is of high interest. For this a fundamental understanding of structure and dynamics on the composition of the ionic liquid is needed. Moreover it is important to analyze of the properties in mixtures with other substances, in particular water. To obtain a better understanding of these properties we perform molecular dynamics simulations. The studied ionic liquids are made of 1-alkyl-3-methylimidazolium cations and BF<sub>4</sub> or NO<sub>3</sub> anions and contain water. As in previous studies [1,2] we analyze structure and dynamics on various length scales, but this time for different alkyl chain lengths and water mole fractions. Of special interest are two properties of the mixtures. First, the existence of structural inhomogeneity and second, the transport between different clusters. Thus, our approach enables detailed insights into structure-dynamics relations in ionic liquids.

[1] Pal, T. *et al.*, *ChemPhysChem*, 18 (16), **2017**

[2] Pal, T. *et al.*, *J. Chem. Phys.*, 150 (12), **2019**

CPP 16.12 Wed 15:00 CPPa

**Correlation Length in Concentrated Electrolytes: Insights from All-Atom Molecular Dynamics Simulations** — SAMUEL W. COLES<sup>1</sup>, •CHANBUM PARK<sup>2,3</sup>, ROHIT NIKAM<sup>2,3</sup>, MATEJ KANDUČ<sup>2,4</sup>, JOACHIM DZUBIELLA<sup>2,5</sup>, and BENJAMIN ROTENBERG<sup>1</sup> — <sup>1</sup>Sorbonne Université, CNRS, Physicochimie des électrolytes et nanosystèmes interfaciaux, UMR PHENIX, 4 pl. Jussieu, F-75005, Paris, France — <sup>2</sup>Research Group for Simulations of Energy Materials, Hahn-Meitner-Platz 1, D-14109, Berlin, Germany — <sup>3</sup>Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489, Berlin, Germany — <sup>4</sup>Jožef Stefan Institute, Jamova 39, SI-1000, Ljubljana, Slovenia — <sup>5</sup>Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, D-79104, Freiburg, Germany

We study the correlations length of the charge-charge pair correlations in concentrated electrolyte solutions by means of all-atom, explicit-solvent molecular dynamics simulations. We investigate LiCl and NaI in water, as well as two more complex, molecular electrolyte systems of LiTFSI, in water and in DME/DOL. We observe a Debye-Hückel like regime at low concentration, followed by a minimum reached when  $d/\lambda_D \approx 1$ , where  $\lambda_D$  is the Debye correlation length and  $d$  the effective ionic diameter, and an increasing correlation length with salt concentration in very concentrated electrolytes. As in the experiments, we find that the screening length in the concentrated regime follows a universal scaling law as a function  $d/\lambda_D$  for all studied salts. However, the scaling exponent is significantly lower than the experiments.

## CPP 17: Theorie and Simulation - organized by Jens-Uwe Sommer (Leibniz-Institut für Polymerforschung Dresden, Dresden) (joint session CPP/DY)

Time: Wednesday 9:00–14:40

Location: CPPb

**Invited Talk**

CPP 17.1 Wed 9:00 CPPb

**Data-driven methods in polymer physics: exploring the sequence space of copolymers** — ●MARCO WERNER — Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany

Automated experiments and computer simulation on highly parallel machines push the limits of available data in the field of soft matter. For long polymer chains, however, any data set can cover only a marginal fraction of the giant chemical space and conformation space involved. In this talk, data-driven strategies are discussed that allow to trace hidden physical patterns in both giant spaces by machine learning algorithms. The discussion is centered on the example of hydrophilic / hydrophobic copolymers and their interaction with lipid membranes. A neural network has been trained to predict the free energy landscape near a membrane as a function of the copolymer sequence. The information learned in the hidden neural layers showed that the neural network compressed the sequence space into physically meaningful latent variables. The learned semantics was transferable between simulation data with different levels of coarse-graining, and allowed for a physics-informed inverse search for the copolymer sequence leading to the smallest translocation time through the membrane.

CPP 17.2 Wed 9:40 CPPb

**Prediction of iSCFT chemical potentials via machine learning** — ●LUCIA MILENA WESENBERG, LUDWIG SCHNEIDER, and MARCUS MÜLLER — Institute for Theoretical Physics, Georg-August University Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

We explore the use of machine learning to enhance the simulation of polymeric nanostructures. Self-assembly of symmetric diblock copolymers is the chosen testing system for this purpose. Such polymers consist of two equally long blocks of different monomer types. As the two monomer types are incompatible but linked in the center of each polymer, microphase separation occurs.

Simulations of such systems often pose a challenge for particle-based models as large systems and concomitantly long time scales need to be simulated. Thus, continuum models are employed, where the dynamics can be conceived as the relaxation towards the local minimum of a free-energy basin and jumps between such basins. These models reduce the degrees of freedom by integrating out the molecular degrees of freedom. The most detailed continuum model investigated here is the Self-Consistent Field Theory (SCFT). Unfortunately, dynamic SCFT requires the chemical potential of a non-equilibrium morphology that is computationally expensive to obtain. The SCFT potential calculation is an iterative process, and the stability of the algorithm depends heavily on the starting conditions. Our machine learning approach provides suitable initial conditions for the algorithm. The predicted starting conditions reduce the computational effort considerably.

CPP 17.3 Wed 10:00 CPPb

**Machine Learning Inter-Atomic Potentials Generation Driven by Active Learning: A Case Study for Amorphous and Liquid Hafnium dioxide** — ●ANAND NARAYANAN KRISHNAMOORTHY<sup>1,2</sup>, GANESH SIVARAMAN<sup>3</sup>, MATTHIAS BAUR<sup>1</sup>, CHRISTIAN HOLM<sup>1</sup>, CHRIS BENMORE<sup>6</sup>, MARIUS STAN<sup>4</sup>, GABOR CSANYI<sup>5</sup>, and ÁLVARO VÁZQUEZ-MAYAGOITIA<sup>7</sup> — <sup>1</sup>Institute for Computational Physics, University of Stuttgart — <sup>2</sup>Helmholtz Institute Muenster — <sup>3</sup>Leadership Computing Facility, Argonne National Laboratory - USA — <sup>4</sup>Applied Materials Division, Argonne National Laboratory, USA — <sup>5</sup>Department of Engineering, University of Cambridge, UK — <sup>6</sup>X-ray Science Division, Argonne National Laboratory, USA — <sup>7</sup>Computational Science Division, Argonne National Laboratory, USA

We propose a novel active learning scheme for automatically sampling a minimum number of uncorrelated configurations for fitting the Gaussian Approximation Potential (GAP). We apply this scheme to a Hafnium dioxide (HfO<sub>2</sub>) dataset generated from a melt-quench ab initio molecular dynamics (AIMD) protocol. Our results show that the active learning scheme, with no prior knowledge of the dataset is able to extract a configuration that reaches the required energy fit tolerance. Further, molecular dynamics (MD) simulations performed using this active learned GAP model on 6144-atom systems of amorphous and liquid state elucidate the structural properties of HfO<sub>2</sub> with near

ab initio precision and quench rates (ie 1.0 K/ps) not accessible via AIMD.

**40 min. meet the speakers - break**

CPP 17.4 Wed 11:00 CPPb

**BoltzmaNN: Heuristic inverse design of pair potentials using neural networks** — ●FABIAN BERRESSEM, MIHIR KHADILKAR, and ARASH NIKOUBASHMAN — Institute of Physics, Johannes Gutenberg University Mainz, Germany

In this work, we investigate the use of neural networks (NNs) to devise effective equations of state from a given isotropic pair potential using the virial expansion of the pressure. We train the NNs with data from molecular dynamics simulations, sampled in the NVT ensemble at densities covering both the gas- and liquid-like regime. We find that the NNs provide much more accurate results compared to the analytic estimate of the second virial coefficient derived in the low density limit. Further, we design and train NNs for computing the potential of mean force from the radial pair distribution function,  $g(r)$ , a procedure which is often performed for coarse-graining applications. Here, we find that a good choice for the loss function is crucial for an accurate prediction of the pair potentials. In both use cases, we study in detail how providing additional information about forces and the density impacts the performance of the NNs. We find that including this additional information greatly increases the quality of the predictions, since more correlations are taken into account. Further, the predicted potentials become smoother and are in general much closer to the target potential.

CPP 17.5 Wed 11:20 CPPb

**PolyEC - an event-chain framework** — ●TOBIAS A. KAMPMANN, DAVID MÜLLER, and JAN KIERFELD — TU Dortmund University, Germany

PolyEC is a MC event chain framework suitable for simulation of various colloidal systems. We focus on modularity and extensibility to simulate heterogeneous systems. In event-chain simulations only one particle is active and interactions can be treated independently by factorization, which allows for a highly modular approach for particle-based simulations. Albeit ECMC is a monte-carlo method, a single event-chain is deterministic (although there are modifications where this is not true). One crucial feature of this method is that each state a piece-wise deterministic event-chain visits between events are properly (Boltzmann-) weighted. This opens the possibility to measure observables like pressure or the distribution of energy on the fly. As examples we show needle-colloid mixtures and an active particle system.

**Invited Talk**

CPP 17.6 Wed 11:40 CPPb

**Structure formation in drying films and droplets** — ●ARASH NIKOUBASHMAN<sup>1</sup>, MICHAEL HOWARD<sup>2</sup>, MICHAEL KAPPL<sup>3</sup>, and HANS-JÜRGEN BUTT<sup>3</sup> — <sup>1</sup>Johannes Gutenberg University Mainz, Mainz, Germany — <sup>2</sup>Auburn University, Auburn (AL), USA — <sup>3</sup>Max Planck Institute for Polymer Research, Mainz, Germany

Drying complex liquids are encountered in many technologies, including painting, manufacturing polymer LED displays, and spraying pesticides. Here, colloids and/or polymers are typically initially dispersed in a solvent such as water, which then evaporates, leaving behind a dried residue. Our recent simulations and experiments of drying bidisperse suspensions revealed that sufficiently fast evaporation could induce spatial segregation of the two species, with the smaller ones accumulating at the liquid-air interface followed by a homogeneously mixed region of small and big particles. To understand this counterintuitive behavior, we conducted particle-based simulations and dynamic density functional theory calculations, with and without hydrodynamic interactions. According to our model calculations, this drying-induced segregation occurs due to a local increase of the solute concentration near the film-air interface, resulting in a chemical potential gradient for both species; typically, this gradient is steeper for the larger particles, leading to a stronger force pushing them away from the liquid-air interface. Segregation then occurs if the mobility of the larger particles decreases slower than the driving force increases. Comparing the

various simulations and experiments, we found that including hydrodynamics can decrease or even completely suppress the segregation.

CPP 17.7 Wed 12:20 CPPb

**Structure of bottlebrush polymers end-grafted to a planar surface** — ●JAROSLAW PATUREJ<sup>1</sup>, PAUL JUNGMANN<sup>2</sup>, JENS-UWE SOMMER<sup>3</sup>, and TORSTEN KREER<sup>2</sup> — <sup>1</sup>University of Silesia, Katowice, Poland — <sup>2</sup>IPF, Dresden, Germany — <sup>3</sup>Johannes Gutenberg Universität, Mainz, Germany

Polymer brush is a hybrid material composed of a solid substrate coated with end-grafted polymers. We conducted coarse-grained molecular dynamics simulations and scaling theory of the equilibrium structure of planar brushes formed by bottlebrush polymers. Bottlebrushes are branched macromolecules consisting of densely spaced linear side chains grafted along a central (linear) backbone. We elucidate the relationship between bottlebrush architecture, surface coverage  $\sigma$  and polymer brush thickness  $H$ . We study the impact of three length scales on the brush height  $H$ :  $D_0$ , the cross-section radius of bottlebrushes determined by the degree of polymerization of side chains  $N_{sc}$ ,  $R_0$  the (overall) size of bottlebrushes controlled by the degree of polymerization of backbone  $N_{bb}$  and  $d$  the distance between nearest-neighbor tethering sites. The latter quantity provides a measure of molecular coverage  $\sigma$  of a substrate defined as the number of bottlebrush polymers per unit surface area  $\sigma \propto 1/d^2$ . Our theoretical analysis identifies three conformational regimes for the height  $H$ , which gradually establish upon increasing substrate coverage and stem from interplay between relevant length scales:  $d$ ,  $D_0$  and  $R_0$ .

CPP 17.8 Wed 12:40 CPPb

**Thermal conductivity of commodity plastics: From conventional to smart polymers** — ●DEBASHISH MUKHERJI — Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver Canada

Polymers are an important class of soft matter whose properties are dictated by large fluctuations. Because of this reason commodity polymers are ideal for the flexible design of advanced materials. However, applications of polymers are often hindered by their low thermal conductivity  $\kappa$ . While low  $\kappa$  values are desirable for thermoelectric materials, they create severe problems when used under the high temperature conditions. Going from the polymers dictated by weak Van der Waals to hydrogen-bonded interactions,  $\kappa$  varies between 0.1-0.4 W/Km. Using molecular dynamics simulations we study thermal transport and its links to the elastic response of polymers. We find that there exists a maximum attainable stiffness, thus limiting an upper bound of  $\kappa$ . The specific chemical details and the glass transition temperature play no role in controlling  $\kappa$ , especially when the microscopic interaction is hydrogen bonded. These results are consistent with the minimum thermal conductivity model and experiments.

[1] D. Mukherji, C. M. Marques, K. Kremer, Annual Review of Condensed Matter Physics 11, 271 (2020). [2] D. Bruns, T. E. de Oliveira, J. Rottler, D. Mukherji, Macromolecules 52, 5510 (2019). [3] C. Ruscher, J. Rottler, C. Boott, M. J. MacLachlan, D. Mukherji, Physical Review Materials (accepted) (2019).

60 min. meet the speakers - break

CPP 17.9 Wed 14:00 CPPb

**Polymer Architectures by Chain Walking Catalysis - Theory, Simulations, and Experiments** — ●RON DOCKHORN<sup>1</sup>, LAURA PLÜSCHKE<sup>1,2</sup>, ALBENA LEDERER<sup>1,2</sup>, JAN MERNA<sup>3</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — <sup>2</sup>Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — <sup>3</sup>University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Recently developed chain walking catalysis is an elegant approach to synthesize branched polyethylenes (CWPE) with controllable structure and properties. The catalyst is able to walk along the polymer and to polymerize ethylene and  $\alpha$ -olefines into complex topologies depending on pressure, temperature, and olefine concentration introducing branch-on-branch structures. Coarse-grained Monte Carlo simulations utilizing the bond fluctuation model of the CWPE are performed to investigate the influence of the walking mechanism on the polymer architecture. For slow walking rates the structure grows with linear chain extensions, whereas fast walking rates promote dendritic growth of the polymer. The crossover regime is characterized by linear global features and dendritic local substructures contrary to randomly hyperbranched systems. Indeed, the obtained CWPE systems have characteristics of dendritic bottle brushes and the degree of branching can be adjusted by the walking rate of the catalyst. These findings are aimed to understand the physical properties of the CWPE structures and to improve the synthesis of a new class of hyperbranched molecules.

CPP 17.10 Wed 14:20 CPPb

**Mechanics of shape-shifting droplets** — ●IRETH GARCIA-AGUILAR<sup>1</sup>, PIERMARCO FONDA<sup>1</sup>, ELI SLOUTSKIN<sup>2</sup>, and LUCA GIOMI<sup>1</sup> — <sup>1</sup>Instituut-Lorentz, Universiteit Leiden, The Netherlands — <sup>2</sup>Department of Physics and Institute of Nanotechnology & Advanced Materials, Bar-Ilan University, Ramat-Gan, Israel

It has been long understood that dispersed liquid droplets are spherical in order to minimize the tension at their interface. Surprisingly, oil emulsion droplets in water have been observed to spontaneously deform into polyhedral shapes when cooling down the system. The equilibrium shape of a droplet at some temperature depends on its initial volume but all deformations take place below the freezing point of the surfactant monolayer, while the bulk oil and water remain liquid. The frozen interface forms an hexagonal lattice which is topologically constrained to accommodate defects. These produce large stresses that induce in and out-of-plane deformations in the crystal which in turn are opposed by the interfacial tension between oil and water. Initially, it was thought that this competition determines the droplet shape; however, this alone can not explain the size dependence of the deformations. By modeling the interface as a 2D elastic surface and studying its equilibrium geometry, we found a mechanism that explains the size-scaling behaviour. Interestingly, crystalline defects are not the only peculiarity playing a role in shaping the droplets.

## CPP 18: Complex Fluids and Soft Matter 1 (joint session DY/CPP)

Time: Wednesday 9:00–10:30

Location: DYa

CPP 18.1 Wed 9:00 DYa

**Flow structure of marangoni-contracted sessile droplets** — O. RAMIREZ<sup>1</sup>, M.A. HACK<sup>2</sup>, W. KWIECINSKI<sup>3</sup>, E.S. KOOLJ<sup>3</sup>, T.J. SEEGER<sup>2</sup>, J.H. SNOELJER<sup>2</sup>, and ●S. KARPITSCHKA<sup>1</sup> — <sup>1</sup>MPI for Dynamics and Self-Organization, Göttingen, Germany — <sup>2</sup>Physics of Fluids Group, University of Twente, Enschede, Netherlands — <sup>3</sup>Physics of Interfaces Group, University of Twente, Enschede, Netherlands

A droplet of two miscible liquids should spread over a high-energy surface until complete wetting. However, if one component is more volatile and has a higher surface tension, a quasi-stationary non-vanishing apparent contact angle can be observed. This is caused by the enrichment of the residual component near the contact line and the associated surface tension gradient. A hydrodynamic-evaporative model, using a long-wave approximation for the droplet coupled to diffusion limited evaporation predicts a balance between Marangoni and capillary flows and a power law between the apparent contact angle and the

ambient humidity [Karpitschka et al., Langmuir (2017)]. This explanation differs from a recent model, where the low surface tension of a precursor around the droplet is held responsible [Benusiglio et al., Soft Matter (2018)]. A discrimination between possible mechanisms requires experimental resolution of the flow in the drop. We present uPIV measurements and relate them to the apparent shape of the drop, for aqueous solutions of various short chain carbon diols. Depending on the surface activity of the diol, its concentration, and the ambient humidity, we observe different regimes, indicating that multiple mechanisms lead to the observed angles.

CPP 18.2 Wed 9:20 DYa

**Coalescence of liquid droplets in a quasi 2D liquid film** — ●CHRISTOPH KLOPP, RALF STANNARIUS, and EREMIN ALEXEY — Institute of Physics, Otto von Guericke University, Department of Non-linear Phenomena, 39106 Magdeburg

Coalescence of droplets plays a crucial role in nature and modern tech-

nology. Various experimental and theoretical studies explored droplet dynamics in 3D and on 2D solid or liquid substrates [1-3].

Here, we demonstrate coalescence of isotropic droplets in thin quasi 2D liquids, an overheated smectic A films. We investigated their dynamics experimentally and measured the shape deformation during the whole merging process using high-speed imaging. This system is a unique example, where the lubrication approximation can be directly applied, and the smectic membrane plays the role of the precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared our results with existing models for liquid lens coalescence on liquid and solid surfaces.

[1] J. D. Paulsen et al., Coalescence of bubbles and drops in an outer fluid, *Nat. Commun.* 5, 3182 (2014)

[2] D. G. A. L Aarts et al., Hydrodynamics of Droplet Coalescence, *Phys. Rev. Lett.* 95, 164503 (2005)

[3] N. S. Shuravin et al., Coalescence of viscous two-dimensional smectic islands, *Phys. Rev. E* 99, 062702 (2019)

CPP 18.3 Wed 9:40 DYa

### Designing Pickering Emulsions for Catalysis: Influence of Nanoscale Particle Properties on Microscale Droplets —

•SEBASTIAN STOCK<sup>1</sup>, ANNIKA SCHLANDER<sup>1</sup>, KAI SPANHEIMER<sup>1</sup>, MARESA KEMPIN<sup>2</sup>, ARIANE WEBER<sup>3</sup>, REINHARD SCHOMÄCKER<sup>3</sup>, ANJA DREWS<sup>2</sup>, MARCUS GALLEI<sup>4</sup>, and REGINE VON KLITZING<sup>1</sup> — <sup>1</sup>TU Darmstadt, Darmstadt, Germany — <sup>2</sup>HTW Berlin, Berlin, Germany — <sup>3</sup>TU Berlin, Berlin, Germany — <sup>4</sup>Saarland University, Saarbrücken, Germany

Pickering Emulsions (PEs) describe emulsions stabilized by (nano) particles. The aim of the work was to design PEs as a reaction environment for catalytic reactions. As a model reaction the hydroformylation of 1-dodecene was investigated. Due to the PEs high stability separation methods with outstanding energy efficiency are applicable e.g. the separation of the oil phase by nanofiltration. Many microscopic and macroscopic PE properties are determined in a large degree

by the nanoscale properties of the particles. In order to distinguish the impact of particle surface charge both positively and negatively charged silica spheres were produced. This was achieved by adequate surface modification. The resulting nanoscale particle properties concerning size, shape, charge, and hydrophobicity were investigated via Transmission Electron Microscopy (TEM),  $\zeta$ -potential and sessile drop measurements, the effect on the microscopic emulsion properties were studied with microscopy and the PEs reaction behavior including yield and stability was evaluated.

### Invited Talk

CPP 18.4 Wed 10:00 DYa

**When surface viscosities rule: Bubble relaxation and thin film wrinkling** — •KIRSTEN HARTH — Institut für Physik, Otto von Guericke Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

The dynamics of liquid drops and gas bubbles in a surrounding fluid is a classic field of fluid mechanics, studied for over a century. The mathematical problem can be complex already for the case of clean fluid-fluid interfaces, characterized solely by a constant surface tension. However, applications such as ink-jet printing, emulsion characterization or typical biologically inspired systems usually deal with more complex interfacial properties, e.g., adsorbed fluid or contaminant films. Those can completely dominate the overall shape dynamics.

Merged centimeter-sized soap bubbles or rupturing micrometer-thick soap films are a simple yet ideal model system for surface-tension based relaxation. Replacing the soap film by a more complex membrane, nanometer-thin liquid crystalline films in our case, introduces qualitatively new effects due to reorganization of the membrane upon surface area reduction. The talk highlights two aspects: First, the consequences of an effective interfacial viscosity for the relaxation dynamics, known also from interfacial fluid films or adsorbed surfactant layers. Second, out-of-plane bulging and dynamic wrinkling of the interfacial membrane in response to external stress. Experiments will be accompanied by a theoretical / numerical analysis.

## CPP 19: Glasses and Glass Transition 1 (joint session DY/CPP)

Time: Wednesday 9:30–10:30

Location: DYc

CPP 19.1 Wed 9:30 DYc

### Molecular dynamics study of 1,4-polybutadiene supported films —

•FEDIR DEMYDIUK<sup>1</sup>, HENDRIK MEYER<sup>1</sup>, JOERG BASCHNAGEL<sup>1</sup>, MATHIEU SOLAR<sup>1</sup>, and WOLFGANG PAUL<sup>2</sup> — <sup>1</sup>Institute Charles Sadron, University of Strasbourg, UPR22 CNRS 67034 Strasbourg, France — <sup>2</sup>Institut für Physik, University of Halle, 06120 Halle (Saale), Germany

Our work is dedicated to studying the influence of realistic intrachain constraints imposed due to the presence of torsional barriers on the glass transition in thin polymer films of supported geometry by means of classical molecular dynamics simulations. In order to do so, we use the well-established united-atom model of 1,4-polybutadiene, that has been developed by W. Paul and coworkers (G. D. Smith and W. Paul, *J. Phys. Chem. A*, 102, 1200 (1998)) and studied in confined systems (M. Solar, K. Binder and W. Paul, *J. Chem. Phys.*, 146, 203308 (2017)). In our case, the model had to be adapted for usage in systems with free surface.

Focusing on dynamics of united atoms and shear-stress relaxation, we first discuss our results for bulk polybutadiene and then present first extensions of bulk simulations to supported films. First analysis of the supported films shows that dynamics is enhanced at the free surface and slowed down at the substrate.

CPP 19.2 Wed 9:50 DYc

### Glassy dynamics, glass transition and electrical conductivity of Guanidinium based ILCs: Influence of the cation headgroup configuration —

•MOHAMED A KOLMANGADI, ARDA YILDIRIM, and ANDREAS SCHÖNHALS — Bundesantalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Molecular mobility and conductivity of four bent shaped tetramethylated guanidinium based ionic liquid crystals (ILCs) with varying head group configuration (cyclic or acyclic) and alkyl chain length is investigated by a combination of broadband dielectric spectroscopy (BDS) and specific heat spectroscopy (SHS). BDS investigation reveals two relaxation processes: a localized  $\gamma$  process and  $\alpha 1$  process corresponding

to the glassy dynamics. SHS investigations show one calorimetrically active  $\alpha 2$  relaxation process also corresponding to the glassy dynamics of the system. The temperature dependencies of the relaxation rates of two different glassy dynamics are similar for the cyclic ILC while for the acyclic counterpart they are different. Possible molecular assignments for the  $\alpha 1$  and  $\alpha 2$  relaxation are discussed in detail. Alongside relaxation processes, a significant conductivity contribution was observed for all ILCs, where the absolute value of DC conductivity increases by 4 orders of magnitude at the transition from the crystalline to the hexagonal columnar phase. The increase is traced to the change in the underlying conduction mechanism from the delocalized electrical conduction in the Cry phase to ionic conduction in the quasi 1D ion columns formed in the hexagonal columnar mesophase.

CPP 19.3 Wed 10:10 DYc

### A new approach to probe the plastic rearrangements inside a shear band. —

•MOUMITA MAITI and ANDREAS HEUER — University of Münster, Münster, Germany

We follow a single particle trajectory of a system subjected to a uniform shear by calculating its instantaneous displacement with time. There are intermittent hops in the trajectory, which are treated as plastic events, and the particles which have performed hops, are called active. In the steady state, the number of events per particle of the whole system increases initially by increasing system size, and by further increment the number almost saturates. The onset of saturation is the onset of shear banding. Interestingly, above the onset, we observe a system size scaling in the number of plastic events only inside the shear band. The scaling is explained from the intervals between two consecutive hops of a particle, which decreases on an average with increasing size. We further show that there is a stronger coupling between active particles with increasing system size which helps to understand the smaller value of the intervals, so our approach captures the collective nature of plastic events. Additionally, we observe a system spanning avalanches for these sizes which exhibit shear banding, and the distribution of avalanche sizes have a different exponent from the mean field theory.

## CPP 20: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00

Location: DYa

CPP 20.1 Wed 11:00 DYa

**Thermally driven material transport in thin freestanding films** — •TORSTEN TRITTEL, KIRSTEN HARTH, CHRISTOPH KLOPP, and RALF STANNARIUS — Otto-von-Guericke Universität, 39106 Magdeburg, Germany

In addition to their important role in display applications, liquid crystals are attractive in the field of fundamental physics. Smectics can form thin free-standing films with aspect ratios exceeding one million to one (width/thickness). These homogeneously thin films serve as an ideal model system for the study of two-dimensional hydrodynamics. We investigate thermally driven material transport within the film plane under microgravity conditions. Temperature differences in the film lead to thermocapillary (Marangoni) flow. In materials with a normal (negative) temperature coefficient of the surface tension  $d\sigma/dT < 0$ , temperature inhomogeneities lead to material transport from the warm to the cold film edge. In materials with  $d\sigma/dT > 0$ , flow is reversed. We present a quantitative model, which predicts that the temperature difference between the hot and cold film edge is the relevant parameter, not the gradient as in conventional thermoconvection.

CPP 20.2 Wed 11:20 DYa

**Phase Field Crystal Model of patchy colloids in two dimensions** — •ROBERT F. B. WEIGEL and MICHAEL SCHMIEDEBERG — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Motivated by our recent simulation studies of quasicrystals that occur in systems of patchy colloids [1,2], we develop a Phase Field Crystal Model for such particles. We consider two-dimensional patchy colloids with symmetrically placed attractive sites on their surface, such that they interact with preferred binding angles. We construct a free energy functional that is similar to the free energy used for liquid crystals [3], but obeys the symmetry of the patchy colloids. The functional depends on both a density field and an orientation field. Free numerical minimization of the free energy yields a rich phase behavior of complex structures.

- [1] Gemeinhardt et al., Eur. Phys. J. E 41, 126 (2018).
- [2] Gemeinhardt et al., EPL 126, 38001 (2019).
- [3] Achim et al., Phys. Rev. E 83, 061712 (2011).

CPP 20.3 Wed 11:40 DYa

**Orientational order parameters for arbitrary classical and quantum liquid crystals** — •MICHAEL TE VRUGT and RAPHAEL WITTKOWSKI — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

The orientational order of liquid crystals is measured using orientational order parameters such as the polarization vector and the nematic tensor. These are obtained from an angular or Cartesian multipole expansion of the one-body distribution function of the liquid crystal. In recent years, there has been an increase of interest in particles with general shapes, as well as in so-called “quantum liquid crystals” which are relevant, e.g., in superconductors. However, the standard methods for defining order parameters are not applicable to biaxial particles or quantum systems. In this talk, we discuss how the orientational expansion method can be generalized to particles with arbitrary shape [1] and to quantum soft matter [2]. This provides a unified framework for general classical and quantum liquid crystals.

- [1] M. te Vrugt and R. Wittkowski, AIP Advances 10, 035106 (2020)
- [2] M. te Vrugt and R. Wittkowski, Annalen der Physik 532, 2000266 (2020)

\*Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1

CPP 20.4 Wed 12:00 DYa

**Analytical classical density functionals from an equation learning network** — •SHANGCHUN LIN<sup>1</sup>, GEORG MARTIUS<sup>2</sup>, and

MARTIN OETTEL<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — <sup>2</sup>Max Planck Institute for Intelligent Systems, Tübingen, Germany

We explore the feasibility of using machine learning methods to obtain an analytic form of the classical free energy functional for two model fluids, hard rods and Lennard Jones, in one dimension. The Equation Learning Network proposed in Ref.[1] is suitably modified to construct free energy densities which are functions of a set of weighted densities and which are built from a small number of basis functions with flexible combination rules. This setup considerably enlarges the functional space used in machine learning optimization. As a result in Ref [2], we find a good approximation for the exact hard rod functional. For the Lennard Jones fluid, we let the network learn the full excess free energy functional and the excess free energy functional related to interparticle attractions. Both functionals show a good agreement with simulated density profiles inside and outside the training region.

- [1]G. Martius and C. H. Lampert, arXiv:1610.02995 (2016).
- [2]S.-C. Lin, G. Martius and M. Oettel, JCP 152.2 (2020): 021102.

CPP 20.5 Wed 12:20 DYa

**Particle-resolved topological defects of smectic colloidal liquid crystals in extreme confinement** — •RENÉ WITTMANN<sup>1</sup>, LOUIS CORTES<sup>2</sup>, HARTMUT LÖWEN<sup>1</sup>, and DIRK AARTS<sup>2</sup> — <sup>1</sup>Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — <sup>2</sup>Department of Chemistry, University of Oxford, UK

Hard particles are a standard model for colloidal systems and can be effectively studied within classical density functional theory (DFT). Fundamental mixed measure theory (FMMT) allows to predict the phase behavior of a hard-body fluid solely from the shape of individual particles. Recent experimental advances allow for the synthesis of colloids with a nearly hard interaction that can be analyzed on the single-particle level. Slices of such silica rods confined in a three-dimensional chamber under gravity can be considered a quasi-two-dimensional fluid that exhibits typical liquid-crystal behavior in confinement.

Applying FMMT to hard discorectangles in two dimensions, we study a smectic fluid in extreme complex confinement, where the optimal bulk layer spacing competes with the extrinsic geometric and topological constraints. As a result, we characterize a variety of topologically different states in an annular geometry, also observed in particle-resolved experiments with silica rods. By further comparing the free energy of the different states, naturally provided by our DFT, we map out a topological phase diagram, indicating the stable topology depending on the details of the annular geometry.

Publication: R. Wittmann et al., Nat Commun 12, 623 (2021).

CPP 20.6 Wed 12:40 DYa

**Full phase diagram of continuous-time self-propelled particle models with alignment interaction** — •YINONG ZHAO<sup>1</sup>, PAWEL ROMANCZUK<sup>1</sup>, and CRISTIAN HUEPE<sup>2,3</sup> — <sup>1</sup>Institute of Theoretical Biology, Department of Biology, Humboldt Universität zu Berlin — <sup>2</sup>CHuepe Labs, 2713 West Haddon Ave #1, Chicago, IL 60622, USA — <sup>3</sup>Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, IL 60208, USA

Self-propelled particle (SPP) models are widely used for exploring emergence of collective motion in nature. Despite the significant advances over the past decades in understanding self-organized active matter, many questions remain open about the general phase space of Vicsek-like alignment models and the regions of validity of corresponding analytical theories. We investigate a set of different continuous-time SPP-models with alignment interactions. We find that all these models share qualitatively the same phase diagram. Focusing on one of them, we identify three homogeneous states with long-range orientational order, that can be distinguished using statistical approaches. We tested the predictions of the Toner-Tu theory on these states and show that they do not hold for all three of them. Furthermore, we also phenomenologically explore the role of positional repulsion on the emergent spatial structure. Our study provides a broad, over-arching perspective on continuous-time alignment-based SPP model.

## CPP 21: Glasses and Glass Transition 2 (joint session DY/CPP)

Time: Wednesday 11:00–13:00

Location: DYc

CPP 21.1 Wed 11:00 DYc

**Residual stress distributions and mechanical noise in athermally deformed amorphous solids** — ●CÉLINE RUSCHER<sup>1,2</sup>, DANIEL KORCHINSKI<sup>2</sup>, and JOERG RÖTTLER<sup>2</sup> — <sup>1</sup>Institut Charles Sadron, Strasbourg, France — <sup>2</sup>Department of Physics and Astronomy and Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Amorphous solids are yield stress materials whose flow consists of periods of elastic loading interrupted by rapid stress drops, or avalanches, coming from microscopic rearrangements known as shear transformations (STs). From the microscopic point of view, the density of STs, or density of local residual stresses,  $P(x)$ , governs the statistical properties of global collective failure events at the yielding transition.

Using atomistic simulations, we reveal the evolution of  $P(x)$  upon deformation. A pseudogap form  $P(x) \sim x^\theta$  is observed in the freshly quenched state and in the early stages of deformation. After a few percent strain, however,  $P(x)$  starts to develop a system size dependent plateau in the small  $x$  limit. To explain the origin of the plateau we consider a mesoscopic elastoplastic approach. Our results show how the spatial extent of avalanches in the stationary regime has a profound effect on the distribution of local residual stresses  $x$ . While the entrance into the plateau is set by the lower cutoff of the mechanical noise produced by individual STs, the departure from the usually assumed power-law pseudogap form comes from stress fluctuations induced by collective avalanches.

CPP 21.2 Wed 11:20 DYc

**Evaluation of Local Atomic Structural Changes in  $Cu_{50}Zr_{50}$  Cluster Assembled Metallic Glasses through Molecular Dynamics Simulations** — ●SYAMAL PRANEETH CHILAKALAPUDI<sup>1</sup>, SHYAM KATNAGALLU<sup>1</sup>, WOLFGANG WENZEL<sup>1</sup>, PENGHUI CAO<sup>2</sup>, and HORST HAHN<sup>1,2,3</sup> — <sup>1</sup>Institute Nanotechnology, Karlsruhe Institute of Technology, Germany — <sup>2</sup>Dept. Mat. Sci. & Engg., University of California-Irvine, USA — <sup>3</sup>KIT-TUD Joint Research Laboratory Nanomaterials, Technische Universität Darmstadt, Germany

Cluster assembled metallic glasses (CAMGs), synthesized by cluster (amorphous) ion beam deposition (CIBD), are a prominent bottom-up approach to tailor amorphous structures. Experimental control of amorphous structure and magnetic properties [1] was demonstrated with a custom-made apparatus which offers precise control on the size and the deposition energy of the clusters under ultra high vacuum [2].

To understand the underlying mechanisms of these structural changes in CAMGs, we performed atomistic molecular dynamics simulations of  $Cu_{50}Zr_{50}$  cluster assembly using LAMMPS. Our simulations model the CIBD process and evaluate changes in the local short-range order in CAMGs as a function of the deposition energy of the clusters. We notice the presence of interfacial regions, formed between every adjacent cluster. The interfaces are most prominent in soft-landing cases. We also investigate the effect of quenching rate used to generate the amorphous clusters on CAMGs.

[1] C. Benel et al., *Mat. Horizons*, (2019) 6, 727[2] A. Fischer et al., *Rev. Sci. Instr.* (2015) 86, 023304

CPP 21.3 Wed 11:40 DYc

**X-ray computed tomography of glass foams with tailored hierarchical pore structure** — ●CRISTINE SANTOS DE OLIVEIRA<sup>1</sup>, RICHARD KOHNS<sup>2</sup>, FELIX MEYERHOEFER<sup>2</sup>, SIMON CARSTENS<sup>2</sup>, DIRK ENKE<sup>2</sup>, RALF BORIS WEHRSPHORN<sup>1,3</sup>, and JULIANA MARTINS DE SOUZA E SILVA<sup>1</sup> — <sup>1</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — <sup>2</sup>Institut für Technische Chemie, Universität Leipzig, Germany — <sup>3</sup>Fraunhofer Gesellschaft, München, Germany

Glass foams are materials consisting of a light-weight porous glass structure of special importance in the fields of civil engineering and bio-implants. Typically, their synthesis involves the thermal foaming of a powder mixture of glass with a foaming agent that decomposes at the foaming temperature, resulting in a solid glass skeleton permeated by empty pores. In our work, we synthesized a series of glass foams with a hierarchical pore structure, obtained by combining pores gener-

ated through the foaming of a powdered mixture of silica-based glass,  $MnO_2$  and  $C$  at 815°C, with pores obtained by phase-separation (performed at circa 500°C) followed by acid leaching and washing. Using a combination of mercury intrusion porosimetry,  $N_2$  sorption and X-ray CT at the micro and nanometer scales we observed that slight changes in the preparation procedure resulted in foams with different porosity, surface area, pore size and pore volume. Furthermore, by applying machine learning segmentation to the X-ray CT data it was possible to map inhomogeneities, residues and cracks inside the foam walls.

CPP 21.4 Wed 12:00 DYc

**Decelerated aging in metallic glasses by low temperature thermal cycling** — ●FATHOLLAH VARNIK — ICAMS, Ruhr-University Bochum, Germany

It has been recently proposed that deep temperature cycling of metallic glasses may lead to a rejuvenation and improve their ductility. Here, we investigate this issue via extensive molecular dynamics simulations of a generic model glass former. We disentangle the effects of aging from those of thermal treatment and show that aging is slowed down but not stopped – neither reversed – during thermal cycling. These observations are corroborated further by a survey of energy distribution, which continues narrowing, albeit with a smaller rate. Our results are in qualitative agreement with recent differential scanning calorimetry measurements on different bulk metallic glasses, which show no measurable rejuvenation upon deeply cooled (cryogenic) thermal cycling. This applies both to as-quenched and well-annealed samples.

CPP 21.5 Wed 12:20 DYc

**Glassy dynamics in viscous liquids - Prospects of broadband NMR relaxometry** — ●MANUEL BECHER<sup>1,2</sup>, MICHAEL VOGEL<sup>2</sup>, and ERNST RÖSSLER<sup>1</sup> — <sup>1</sup>Nordbayerisches NMR-Zentrum, Universität Bayreuth, Germany — <sup>2</sup>Institute of Condensed Matter Physics, TU Darmstadt, Germany

As the molecular dynamics of a liquid undergoing a glass transition features a wide range of timescales over many decades, it is beneficial to study these viscous liquids with broadband spectroscopic techniques. Besides well established methods such as dielectric spectroscopy (DS) and depolarized dynamic light scattering (DDLs) covering many decades in time/frequency, also nuclear magnetic resonance (NMR) offers detailed insights in molecular motion ranging from the boiling point of a liquid to its glassy arrest. However, in most recent publications the spectral shape of the main relaxation peak between DS, DDLs and NMR was readressed and the question of universality arised, rendering the prospect of broadband NMR experiments to a new importance. As NMR experiments can provide single-particle correlation functions of the probed molecular moieties, but are usually carried out at a single Larmor-frequency, interest lies in 'broadening' their frequency range. In this talk, ways to access the relaxation spectrum are presented, focussing on field-cycling (FC) NMR. Here, recent advances allow us to evaluate the concept of frequency-time superposition in molecular glass formers. Moreover, making use of NMR's isotope sensitivity, molecular site-dependent measurements are shown to reveal the impact of molecular flexibility on structural relaxation.

CPP 21.6 Wed 12:40 DYc

**The dynamics of a glassforming Lennard-Jones system below the critical mode-coupling temperature** — ●JUERGEN HORBACH — Heinrich Heine-Universitaet, Duesseldorf, Germany

We present molecular dynamics (MD) computer simulations of a poly-disperse glassforming Lennard-Jones model. The equation of state of this model is very similar to that of the Kob-Andersen binary Lennard-Jones (KABLJ) mixture. At a comparable density, also the critical mode coupling temperature is similar as in the KABLJ mixture. Using the swap Monte Carlo technique in combination with MD, we are able to equilibrate supercooled liquids far below the critical mode coupling temperature. We analyze the properties of these deeply supercooled samples with respect to their dynamics in the beta relaxation regime and their response to external shear. In particular, we find the formation of shear bands at sufficiently low shear rates.



## CPP 22: Poster Session III - Charged Soft Matter and Theory and Simulation

Time: Wednesday 16:30–18:30

Location: CPPp

CPP 22.1 Wed 16:30 CPPp

**In-situ investigation of the thermal stability of thermoelectric thin films based on ionic liquid post-treated PEDOT:PSS** — ●ANNA LENA OECHSLE<sup>1</sup>, JULIAN E. HEGER<sup>1</sup>, NIAN LI<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, SIGRID BERNSTORFF<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,3</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — <sup>2</sup>ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — <sup>3</sup>Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

In total around 66% of the global produced primary energy is lost as waste heat, for example from industrial or everyday life processes. Thermoelectric generators, as they enable the direct conversion of a temperature gradient into electrical power, are therefore considered a promising technique to recycle these large amounts of heat waste. Especially, organic thermoelectric polymers are attractive, owning some advantages like low cost, lightness and high mechanical flexibility, low or no toxicity, as well as a usually low thermal conductivity. In our work we research the positive effect of ionic liquid (IL) treatment on the thermoelectric properties of semi-conducting PEDOT:PSS thin films. Therefore, we measure parameters, like the Seebeck coefficient, electrical conductivity, and furthermore examine the inner film morphology with scattering techniques like grazing incidence small angle x-ray scattering (GISAXS). In addition to find the influence of ILs treatment on the morphology-function relation of the PEDOT:PSS thin films, we also investigate the thermoelectric performance stability these films under operation at elevated temperatures.

CPP 22.2 Wed 16:30 CPPp

**Structural and Dynamic Insights in the Conduction of Lithium-Ionic-Liquid Mixtures in Nanoporous MOFs as Solid-State Electrolyte** — MICAELA VAZQUEZ<sup>1</sup>, ●MODAN LIU<sup>2</sup>, ZEJUN ZHANG<sup>1</sup>, ABHINAV CHANDRESH<sup>1</sup>, ANEMAR BRUNO KANJ<sup>1</sup>, WOLFGANG WENZEL<sup>2</sup>, and LARS HEINKE<sup>1</sup> — <sup>1</sup>Institute of Functional Interfaces, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Metal-organic framework (MOF) based separators in Li-ion-battery (LIB) help stabilize the solid electrolyte interphase and strongly affect the battery performance. The mobility and conduction of the Lithium-ion and organic ionic liquids (ILs) in these materials is crucially dependent on the MOF structures and the IL loading factors.

Here, via both experiments and all-atom molecular dynamics (MD) simulations, we observe complex conduction behaviors of Li-IL in the MOF with loading and composition dependence, particularly the presence of Li-ion prevents the conductivity collapse at high IL loading. MD reveals a vehicular transport for the IL and a Grotthuss-like conduction for Li-ions. At small pore fillings, the Li conduction is limited by the large separation between anions. At high pore fillings, the conduction is governed by the bunching of IL. In contrast to the Li-free IL, the bunching effect is attenuated by the formation of charge-neutral Li-anion complexes, which results in a tremendously increased conductivity at maximum filling. This tuning mechanism may contribute to development of advanced batteries.

CPP 22.3 Wed 16:30 CPPp

**Quantitative prediction of charge regulation in peptides and model ampholytes** — ●PETER KOŠOVAN, RAJU LUNKAD, ANASTASIA MURMILIU, PASCAL HEBBEKER, ZDENĚK TOŠNER, and MIROSLAV ŠTĚPÁNEK — Department of Physical and Macromolecular Chemistry, Charles University

Weak ampholytes are ubiquitous in nature and commonly found in artificial pH-responsive systems. However, our limited understanding of their charge regulation and the lack of predictive capabilities hinder the bottom-up design of such systems. Here, we used a coarse-grained model of a flexible polymer with weakly ionisable monomer units to quantitatively analyse the ionisation behaviour of two oligopeptides model ampholytes. Our simulations predict differences in the charge states between oligopeptides and monomeric amino acids, showing that not only electrostatic interactions between charged groups but also conformational flexibility plays a key role in the charge regulation. By comparing our simulations with experimental results from potentiometric titration, capillary zone electrophoresis and NMR, we demon-

strated that our model reliably predicts the charge state of various peptide sequences. Ultimately, our simulation model is the first step towards understanding the charge regulation in flexible ampholytes, and towards predictive bottom-up design of charge-regulating systems.

CPP 22.4 Wed 16:30 CPPp

**Investigating the surface charge of microplastic particles with Colloidal Probe-Atomic Force Microscopy** — ●THOMAS WITZMANN and ANDREAS FERY — Leibniz-Institute of Polymer Research Dresden, Germany

To date, plastic particles have mainly been categorized by polymer type, shape, and size. But there is another important issue arising when investigating microplastic and its interaction with cells. With decreasing size, the surface-volume ratio increases which makes surface properties more important to consider. It is generally believed that the surface properties of the particles influence the cell interaction. Therefore, we investigated un-functionalized polystyrene particles with the size of 3 micrometer with different surface properties of two different manufactures. We found out that the cellular interaction and uptake of microplastic particles (polystyrene) differs for the two particle types. Using Colloidal Probe-Atomic Force Microscopy (CP-AFM) we could show a significant difference in the electric surface properties: homogeneously charged particles vs. heterogeneously charged particles. The heterogeneous surface charge manifests itself in an electrostatic interaction of the particles that depends on the mutual orientation of the particles. CP-AFM is therefore a magnificent tool to obtain additional information\*s about surface charge and its distribution on microplastic particles.

CPP 22.5 Wed 16:30 CPPp

**Investigation of Cononsolvency Phase Transition of Poly(sulfobetaine)-based Diblock Copolymer Thin Films** — ●PEIXI WANG<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, LUCAS P. KREUZER<sup>1</sup>, TOBIAS WIDMANN<sup>1</sup>, SUZHE LIANG<sup>1</sup>, ROBERT CUBITT<sup>2</sup>, ANDRÉ LASCHEWSKY<sup>3</sup>, CHRISTINE M. PAPADAKIS<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>Technische Universität München, Garching, Germany — <sup>2</sup>Institut-Laue-Langevin, Grenoble, France — <sup>3</sup>Universität Potsdam, Potsdam-Golm, Germany

Co-nonsolvency occurs if a mixture of two good solvents causes the collapse or demixing of polymers into a polymer-rich phase in a certain range of compositions of these two solvents. The non-ionic thermo-responsive polymer, poly(N-isopropylmethacrylamide) (PNIPMAM), has been widely used to investigate its collapse transition behavior in a mixture of two competing good solvents. However, co-nonsolvency response of its block copolymer containing the zwitterionic poly(sulfobetaine)s, especially poly(4-((3-methacrylamidopropyl)dimethylammonio)butane-1-sulfonate)) (PSBP), shows a strong swelling transition in aqueous media, is newly studied. We focus on the co-nonsolvency behavior of PSBP-b-PNIPMAM thin films in water/acetone mixtures by in situ time-of-flight neutron reflectometry (TOF-NR) and spectral reflectance (SR). Furthermore, Fourier transform infra-red (FTIR) spectroscopy is applied to investigate the interactions between the polymer thin film and water/co-solvent, which strongly alters depend on their deuteration level.

CPP 22.6 Wed 16:30 CPPp

**ToF-NR investigation of cononsolvency in PNIPAM-based block-copolymer thin films** — ●CHRISTINA GEIGER<sup>1</sup>, JULIJA REITENBACH<sup>1</sup>, LUCAS P. KREUZER<sup>1</sup>, TOBIAS WIDMANN<sup>1</sup>, PEIXI WANG<sup>1</sup>, ROBERT CUBITT<sup>2</sup>, CRISTIANE HENSCHEL<sup>3</sup>, ANDRÉ LASCHEWSKY<sup>3</sup>, CHRISTINE M. PAPADAKIS<sup>4</sup>, and CHRISTINA GEIGER<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — <sup>2</sup>Institut Laue-Langevin, 38000 Grenoble, France — <sup>3</sup>Fraunhofer-Institut für Angewandte Polymerforschung, 14476 Potsdam, Germany — <sup>4</sup>TU München, Physik-Department, Physik weicher Materie, 85748 Garching

The diblock copolymer PMMA-b-PNIPAM forms micelles in aqueous solution that exhibit a reversible shell collapse transition at the lower critical solution temperature (LCST). Apart from a temperature stimulus, the collapse can be induced by the addition of organic co-solvents due to the competitive attachment and detachment of wa-

ter and co-solvent to the PNIPAM chains. We demonstrate that the co-nonsolvency effect is transferrable from solutions to thin film systems. The film swelling and contraction kinetics due to the uptake of water and co-solvent via solvent vapors are investigated with a focus on time-of-flight neutron reflectometry (ToF-NR). Sequential contrasting experiments using protonated and deuterated compounds are performed to differentiate between the distributions of water and co-solvent within the polymer films.

CPP 22.7 Wed 16:30 CPPp

**Layer-by-layer Spray-coating of Cellulose Nanofibrils and Silver Nanoparticles for Hydrophilic Interfaces** — ●QING CHEN<sup>1,2</sup>, CALVIN BRETT<sup>1,3</sup>, ANDREI CHUMAKOV<sup>1</sup>, MARC GENSCH<sup>1,4</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, VOLKER KÖRSTGENS<sup>4</sup>, DANIEL SÖDERBERG<sup>3</sup>, ANTON PLECH<sup>5</sup>, PENG ZHANG<sup>6</sup>, PETER MÜLLER-BUSCHBAUM<sup>4</sup>, and STEPHAN ROTH<sup>1,3</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — <sup>2</sup>University of Science and Technology of China, 230026 Hefei, China — <sup>3</sup>KTH Royal Institute of Technology, 10044 Stockholm, Sweden — <sup>4</sup>Technische Universität München, 85748 Garching, Germany — <sup>5</sup>Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — <sup>6</sup>Sun Yat-sen University, 510275 Guangzhou, China

Silver nanoparticles (AgNPs) and AgNP-based composite materials have attracted growing interest due to their structure-dependent optical, electrical, catalytic and stimuli-responsive properties. In this work, the fabrication of AgNP/cellulose nanofibril (CNF) thin-films via layer-by-layer (LBL) spray-coating is reported. The CNF substrate contributes to a more uniform distribution of AgNPs by its network structure, and by absorbing the partially dissolved AgNP agglomerates. Our approach provides a platform for a scalable production of AgNP/CNF films with low agglomeration rate by two different methods: (1) multi-step layer-by-layer (LBL) spray coating; and (2) direct spray coating of the AgNP/ CNF mixture. We also obtained a uniform AgNP layer with tailorability and plasmonic properties, suggesting their potential applications in anti-fouling coatings and label-free biosensors.

CPP 22.8 Wed 16:30 CPPp

**Charge-Dependent Microphase Separation in Thin Films from a Multiresponsive Pentablock Quaterpolymer** — ●FLORIAN A. JUNG<sup>1</sup>, DORTHE POSSELT<sup>2</sup>, DETLEF-M. SMILGIES<sup>3</sup>, PANAYIOTA A. PANTELI<sup>4</sup>, CONSTANTINOS TSITSILIANIS<sup>5</sup>, COSTAS S. PATRICKIOS<sup>4</sup>, and CHRISTINE M. PAPADAKIS<sup>1</sup> — <sup>1</sup>Physics Department, Soft Matter Group, Technical University of Munich, Garching, Germany — <sup>2</sup>Department of Science and Environment, Roskilde University, Roskilde, Denmark — <sup>3</sup>Wilson Laboratory, Cornell University, Ithaca, USA — <sup>4</sup>Department of Chemistry, University of Cyprus, Nicosia, Cyprus — <sup>5</sup>Department of Chemical Engineering, University of Patras, Greece

Multiblock copolymers and block copolymers with charged segments are attractive candidates for tunable self-assembly of complex morphologies, but their understanding is still at an early stage. In this contribution, we present an investigation of the self-assembly behavior of a pentablock quaterpolymer with (C-*co*-D)-A-B-A-(C-*co*-D) architecture containing ionizable A blocks in thin films using grazing-incidence small-angle X-ray scattering (GISAXS). The two-dimensional scattering patterns were analyzed using simulations combined with a multi-step fitting procedure. Furthermore, we performed in-situ swelling experiments to explore the impact of solvents with different selectivities and polarities on the morphology. We find that varying the degree of ionization of the ionizable blocks allows altering of the segregation strength between the blocks. The nature of the solvent used for swelling gives the opportunity to tune the structures in a wide range.

CPP 22.9 Wed 16:30 CPPp

**Hybrid Energy Harvester based on Triboelectric Nanogenerator and Solar Cell** — ●TIANXIAO XIAO<sup>1</sup>, WEI CHEN<sup>1</sup>, WEI CAO<sup>1</sup>, STEPHAN V. ROTH<sup>2,3</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,4</sup> — <sup>1</sup>TUM, Garching, Germany — <sup>2</sup>DESY, Hamburg, Germany — <sup>3</sup>KTH, Stockholm, Sweden — <sup>4</sup>MLZ, Garching, Germany

Developing clean energy lies the heart of sustainable development of human society. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easily fabricated, TENG has become one of the most promising candidates in replacement of conventional fossil fuels and attracted worldwide attention in

the past years. However, to further increase the energy harvesting efficiency and broaden application fields, integrating the TENG with other kinds of energy harvesters in one device is a possible way to meet these needs. In the present work, a TENG based hybrid energy harvester is designed and fabricated on the flexible polyethylene terephthalate (PET) substrate. This hybrid device consists of a single-electrode mode TENG component and a PbS quantum dots (QDs) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 22.10 Wed 16:30 CPPp

**Dynamics in polymer-fullerene blends for photovoltaic applications** — ●DOMINIK SCHWAIGER<sup>1</sup>, WIEBKE LOHSTROH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching — <sup>2</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed and excitons are created. After diffusion to a donor-acceptor interface, the excitons are dissipated and charge carriers can be extracted from the electrodes. A promising low-bandgap electron donor material is the conjugated polymer PTB7. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, the fullerene derivate PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching). Hydrogen dynamics of pure compounds as well as the blend films are investigated on a pico- to nanosecond timescale in a temperature range from 150 K to 400 K. Results are set into context of photovoltaic performance studies and increase the knowledge base, which is needed for the design of new materials to push the field of organic photovoltaics.

CPP 22.11 Wed 16:30 CPPp

**CNF thin films as sustainable carrier material and their functionalization for energy applications** — ●MARIE BETKER<sup>1,2</sup>, CONSTANTIN HARDER<sup>1,3</sup>, MARC GENSCH<sup>1,3</sup>, CALVIN BRETT<sup>1,2</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, ANDREI CHUMAKOV<sup>1</sup>, QING CHEN<sup>1</sup>, DANIEL SÖDERBERG<sup>2</sup>, and STEPHAN ROTH<sup>1,2</sup> — <sup>1</sup>Deutsches Elektronen Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany — <sup>2</sup>KTH Royal Institute of Technology, Teknikringen 8, 10044 Stockholm, Sweden — <sup>3</sup>Physik-Department E13, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany

Sustainable carrier materials will play an important role in the design of future functional items. One matching candidate for that purpose are cellulose nanofibrils (CNF) with their many beneficial properties: It is lightweight, transparent, flexible and recyclable, and can therefore be used as template for thin-film applications. Spray deposition is a suitable technique to fabricated thin, homogeneous films of large scale and with a ultra-low roughness, which make it fitting for industrial applications. It can also be used to functionalize and thus to implement functional, nanostructured films and multi-component systems. The deposition of conductive silver nanowires as flexible electrodes, poly(3,4-ethylenedioxythiophene) polystyrene sulfonate as blocking layer and of the photoactive layer poly(3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methylester on nanostructured CNF thin films was studied in situ using GISAXS. Important insights into possible templating effects of CNF and into the interactions between the CNF-layers and the functional materials could be gained.

CPP 22.12 Wed 16:30 CPPp

**Oxygen plasma effects on the nanoscale morphology of polyzwitterion-gold interfaces during gold sputtering** — ●APOSTOLOS VAGIAS<sup>1,2</sup>, SIMON J. SCHAPER<sup>1</sup>, JULIAN E. HEGER<sup>1</sup>, YUQIN ZOU<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>3</sup>, MARC GENSCH<sup>1,3</sup>, ANDRÉ LASCHEWSKY<sup>4,5</sup>, STEPHAN V. ROTH<sup>3,6</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,2</sup> — <sup>1</sup>Fachgebiet Physik weicher Materie/Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — <sup>2</sup>Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — <sup>3</sup>Deutsches Elektronen-Synchrotron (DESY), D-22607 Hamburg, Germany — <sup>4</sup>Institut für Chemie, Universität Potsdam, 14476 Potsdam-Golm, Germany — <sup>5</sup>Fraunhofer Institut für Angewandte Polymerforschung IAP,

14476 Potsdam-Golm, Germany — <sup>6</sup>Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Sulfobetaine-based polyzwitterions are efficient interlayers for organic photovoltaics, but their polymer-metal interfacial morphology remains elusive. Moreover, plasma pretreatment of organic solar cells can bypass operational degradation from prolonged light exposure. By in-situ grazing incidence small angle X-ray scattering, we probe the evolution of gold cluster growth on thin polysulfobetaine films during metal sputtering, the latter being an industrially-relevant metal deposition technique. We present differences on the sputtered gold nanostructural morphology with and without oxygen plasma pretreatment.

CPP 22.13 Wed 16:30 CPPp

**Morphology investigation of the active layer of hybrid solar cells with TOF-GISANS** — •VOLKER KÖRSTGENS<sup>1</sup>, LAUTARO DIAZ PIOLA<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, JULIAN HEGER<sup>1</sup>, LUCAS KREUZER<sup>1</sup>, ANNA-LENA OECHSLE<sup>1</sup>, TOBIAS WIDMANN<sup>1</sup>, MATTHIAS NUBER<sup>2</sup>, KLARA STALLHOFER<sup>2</sup>, GAETANO MANGIAPIA<sup>3</sup>, HRISTO IGLEV<sup>2</sup>, REINHARD KIENBERGER<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — <sup>2</sup>TU München, Physik Department, LS Laser- und Röntgenphysik, James-Frank-Str. 1, 85748 Garching — <sup>3</sup>Helmholtz-Zentrum Geesthacht am Heinz Maier-Leibnitz Zentrum, Lichtenbergstr. 1, 85747 Garching

One aspect for the development of non-conventional solar cells should be the sustainability of the production process of devices. Following this idea, we developed hybrid solar cells which can be processed out of aqueous solution. The active layer of these devices is based on laser-processed titania nanoparticles dispersed in a water-soluble thiophene-based polyelectrolyte. The active layers were produced with two of the most common deposition techniques: spray deposition and slot die coating. With these techniques the thickness of layers can be easily controlled and the scale-up toward the coating of large areas is done with low effort. We investigated the morphology of the deposited active layers with time of flight - grazing incidence small angle neutron scattering (TOF-GISANS). The difference of the morphology of these layers is presented and its impact on the performance of devices is discussed.

CPP 22.14 Wed 16:30 CPPp

**In-situ GISAXS Investigation of Sprayed Drugs on a Cellulose Based Matrix** — •ELISABETH ERBES<sup>1,2</sup>, NAIREETA BISWAS<sup>1,2</sup>, STEPHAN V. ROTH<sup>1,3</sup>, SIMONE TECHERT<sup>1,2</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, CALVIN BRETT<sup>1,6</sup>, JOSE VELAZQUEZ GARCIA<sup>1</sup>, SREEVIDYA THEKKU VEEDU<sup>1</sup>, KORNELIYA GOORDEYEVA<sup>3</sup>, ANDREI CHUMAKOV<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>4,5</sup> — <sup>1</sup>DESY, 22607 Hamburg, Germany — <sup>2</sup>Institute for X-ray Physics, Goettingen University, 37077 Goettingen, Germany — <sup>3</sup>Department of Fibre and Polymer Technology, KTH, 100 44 Stockholm, Sweden — <sup>4</sup>Department of Physics, Technical University Munich, 85748 Garching, Germany — <sup>5</sup>MLZ, Technical University Munich, 85748 Garching, Germany — <sup>6</sup>Department of Mechanics, KTH, 100 44 Stockholm, Sweden

These experiments show the first steps to a novel drug carrier strategy for a controlled dosage of anti-COVID-19 drugs. The drugs were embedded into a matrix made of a mixture of hydrophilic carboxymethylated nanocellulose (CMC) hydrogel and disordered hydrophobic peptide hydrogel (P). This gives the opportunity to vary the local uptake in hydrophobic or hydrophilic compartments in the matrix. The structural intercalation and the time-resolved process were investigated with in-situ grazing incidence small angle X-ray scattering (GISAXS) experiments. By using the spraying technique the drug concentration can be tuned for a personalized treatment of the patients. This poster focuses only on the structural change analysis of the CMC fibers. For the analysis of the peptide part please see the poster of Naireeta Biswas.

CPP 22.15 Wed 16:30 CPPp

**Wrinkled Functional Hybrid Multilayers Between Order and Disorder** — •LUKAS WOLFRAM<sup>1</sup>, REGINE FRANK<sup>1,2</sup>, and THOMAS FUHRMANN-LIEKER<sup>1</sup> — <sup>1</sup>Institute of Chemistry, University of Kassel, Germany — <sup>2</sup>Department of Physics and Astronomy, Rutgers, the State University of New Jersey, USA

Multilayer systems of thin films give the opportunity to produce self-structured surfaces via thermal annealing. The corrugations build, so-called wrinkles, are directional isotropic. Wrinkles can be compared to the surface structure of raisins, compressed tissues, or mountain

ranges. A possible application for these structures in thin film technology is the use as a periodic random resonator [1] or previously shown by N.M. Hoinka with spiro compounds.

This Poster will present the first results in testing for a proper material system. So far, experiments with spiro bilayers showed wrinkling over a wide range of surface area. The use of a metallic layer sputtered in a magnetic field can be used to align wrinkles parallel in such a system. My work concentrates on the conditions causing random lasing in these systems and whether there is any systematic correlation existing between the sample morphology and the spectrum observed. For this purpose, python scripts were written to analyse the shape of the corrugation and their directionality to correlate them with imaged spectra in the future.

[1] Shen, Z. *et al.*, Appl. Phys. Lett. 105, 021106, (2014).

[2] N. M. Hoinka, Doctoral Thesis, 2020.

CPP 22.16 Wed 16:30 CPPp

**Co-nonsolvency-type behavior of a poly(sulfobetaine) and a poly(N-isopropylmethacrylamide) thin film in water / methanol vapor** — •LUCAS P. KREUZER<sup>1</sup>, CHRISTOPH LINDENMEIER<sup>1</sup>, CHRISTINA GEIGER<sup>1</sup>, TOBIAS WIDMANN<sup>1</sup>, VIET HILDEBRAND<sup>2</sup>, ANDRÉ LASCHEWSKY<sup>2</sup>, CHRISTINE M. PAPADAKIS<sup>1</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — <sup>2</sup>Universität Potsdam, Institut für Chemie, 14476 Potsdam Golm

The behavior of a poly(sulfobetaine) (PSPE) and a poly(Nisopropylmethacrylamide)(PNIPMAM) thin film in pure water and in mixed water/methanol vapor is studied in-situ with spectral reflectance and Fourier-transform infrared spectroscopy. While PSPE is insoluble in methanol, PNIPMAM is soluble but exhibits a co-nonsolvency behavior in water/methanol mixtures. In thin film geometry, both the PSPE and PNIPMAM swell in pure water vapor, while upon methanol addition, they contract. Their behavior differs significantly regarding the amount of absorbed water in pure water vapor, and the contraction mechanism in mixed water/methanol vapor. The PSPE thin film shows an abrupt one-step contraction, while the PNIPMAM contraction occurs in two steps. When changing to a pure methanol vapor, both, the PSPE and PNIPMAM thin film, show a higher swelling degree than in mixed water/methanol vapor, which indicates a co-nonsolvency-type behavior in polymer thin films.

CPP 22.17 Wed 16:30 CPPp

**Pore-network model for polymer electrolyte membranes** — •PETER BERG and PHILIPPE NADON — Department of Science, University of Alberta

A random pore-network model for polymer electrolyte membranes (PEM) is presented that couples the flow of protons and water through cylindrical channels (bonds) to the swelling of the membrane. While the flows are determined by closed-form solutions of the Poisson-Nernst-Planck-Stokes equations, the fluid-structure interaction is described by a pressure balance at the channel walls. Macroscopic membrane properties, such as the conductivity, permeability and electro-osmotic coefficient, are computed and compared to experimental data in the literature. In light of the model simplifications, the results compare favourably to data but they also point to the importance of describing proton diffusion in PEM nanopores accurately

CPP 22.18 Wed 16:30 CPPp

**Coarse-grained MD simulations of nanoplastic particles interacting with a non-polar environment in aqueous solution** — •LORENZ DETTMANN, ASHOUR AHMED, and OLIVER KÜHN — University of Rostock, Albert-Einstein-Str. 23-24, 18059 Rostock

Plastic waste in form of small particles is an emerging threat for marine and terrestrial ecosystems. Little is known about the fate and potential impacts of plastic nanoparticles in the environment. In this work, an attempt for understanding the molecular level interaction behavior between nanoplastics (NPs) and non-polar environments in aqueous solution is introduced. Here, NPs are simulated with different polymers, namely polyethylene oxide (PEO), polyethylene (PE), polypropylene (PP) and polystyrene (PS). On the other hand, carbon nanotubes (CNTs) are used to mimic non-polar environmental molecular systems. Moreover, hydrophobicity of CNTs is modified by introducing different hydrophobic and hydrophilic functional groups into the inner surface of CNTs. The interaction of the modeled NPs with bare and modified CNTs in the presence of water is investigated via MARTINI force field based coarse-grained molecular dynamics simulations. The results show that hydrophobic polymers have a relatively

strong affinity to CNTs, especially PE. The hydrophobic functional groups introduced into CNTs increased the interaction between hydrophobic polymers and CNTs. In contrast, PEO showed the lowest affinity towards CNTs. Therefore, one can expect that hydrophobic polymers have a higher tendency to accumulate at non-polar environmental molecular systems.

CPP 22.19 Wed 16:30 CPPp

**A mesoscopic approach to magnetostriction of magnetic gels and elastomers** — ●LUKAS FISCHER and ANDREAS M. MENZEL — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our focus is on magnetic gels and elastomers, consisting of rigid magnetizable particles embedded in an elastic polymeric environment. While the particles are discrete objects on the mesoscopic scale, the polymeric body represents an elastic continuum. When magnetized, the particles are subject to magnetic forces and push against the polymeric environment, inducing macroscopic magnetostrictive distortions.

Using analytical theory and numerical evaluations, we determine the overall distortion resulting for different discrete particle arrangements enclosed by a finite-sized, linearly elastic sphere [1–3]. Overall changes in volume and shape are evaluated. In contrast to many other approaches, our formalism includes the basically infinite number of internal degrees of freedom of deformation of the elastic environment.

We assume well-separated particles, all identically magnetized from outside. Depending on the particle arrangement and the compressibility of the elastic material, overall contraction or elongation along the magnetization axis results [1]. Twisted particle structures can lead to overall twist deformations [2], while targeted positioning of particles of different size can tune the overall response [3]. We presume that our approach can support the design of magnetostrictive actuation devices. [1] L. Fischer and A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019). [2] L. Fischer and A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2021). [3] L. Fischer and A. M. Menzel, *Smart Mat. Struct.* **30**, 014003 (2021).

CPP 22.20 Wed 16:30 CPPp

**In situ GISAXS Observation of Sputter-Deposited Gold Nanostructure on Mesoporous Titanium Dioxide Template** — ●SUZHE LIANG<sup>1</sup>, WEI CHEN<sup>1</sup>, SHANSHAN YIN<sup>1</sup>, SIMON J. SCHAPER<sup>1</sup>, THOMAS STRUNKUS<sup>2</sup>, MATTHIAS SCHWARTZKOPF<sup>3</sup>, STENPHAN V. ROTH<sup>3,4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>TU München, Garching, Germany — <sup>2</sup>CAU, Kiel, Germany — <sup>3</sup>DESY, Hamburg, Germany — <sup>4</sup>KTH, Stockholm, Sweden — <sup>5</sup>Heinz Maier-Leibniz Zentrum (MLZ), TU München, Garching, Germany

Gold/titanium dioxide (Au/TiO<sub>2</sub>) nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. Compared to chemical synthesis and lithography, sputter deposition is a facile and scalable method to produce metallic thin films and nanoparticles on substrates in precise controllability. Using nanostructured templates, ordered metal nanostructures were achieved through the sputter deposition approach. Herein, we propose a strategy to fabricate nanostructured Au/TiO<sub>2</sub> hybrid thin films by sputter-depositing Au on mesoporous TiO<sub>2</sub> template. The mesoporous TiO<sub>2</sub> template is prepared by a typical sol-gel synthesis approach with the assistance of diblock copolymer (PS-b-PEO). In order to investigate the kinetics of the sputter-deposited Au growth on the TiO<sub>2</sub> template, in situ grazing-incidence small-angle X-ray scattering (GISAXS) during sputter deposition is measured.

CPP 22.21 Wed 16:30 CPPp

**Modeling and molecular dynamics studies on induced helical polymers** — ●MONTERRAT PENALOZA-AMION and WOLFGANG WENZEL — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Helical conformation plays an important role in biological functions, such as recognition, catalysis and structural support of superstructures. Synthetic helical polymers depend on their inversion barrier and obtaining structural information of dynamic helical polymers requires advanced experimental techniques. Yashima et.al. showed that chiral amines can induce one-handed helical structure in stereoregular cis-transoid poly((4-carboxyphenyl)acetylene) (poly-1), showing intense bands of circular dichroism (CD). Helical models were created based on poly-1. Scan calculations over the dihedral backbone using density functional theory (DFT) on dimers and tetramers of poly-1 backbone were performed to understand the helicity. From these results, Counterclockwise twist with values of -41 and 130 degrees (CCW), and Clockwise twist with values of 42 and -134 degrees (CW) for backbone dihedral were obtained. Molecular Dynamics simulations were per-

formed for 20 ns for both helical models of 20mer with chiral amines and DMSO. Our results show lowest values for RMSD for complexes polymer-R2(CCW) with 0.942 Å, and polymer-S3(CW) with 1.654 Å corresponding to the systems with higher CD intensity in the work of Yashima et.al and indicating that R2 chiral amines could induce a CCW conformation and S3 chiral amines a CW conformation on poly-1.

CPP 22.22 Wed 16:30 CPPp

**Co-nonsolvency effect on phase segregation of polymer solution** — ●ZAHRA MOHAMMADYARLOO and JENS-UWE SOMMER — Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden

Phase segregation of polymer solution in the presence of cosolvent (CNS) is studied by molecular dynamics simulations, where CNS particles are preferential solvent for the polymers. Simulation results for different attraction strengths are compared with the prediction of the adsorption-attraction mean-field theory under constant osmotic pressure. The osmotic pressure has been simulated by a semi-permeable wall in the simulation box. The polymer solution without cosolvent was prepared in the semi-dilute state. Polymer concentration increases until reach a peak by adding more CNS particles, then decreases in higher concentrations of CNS. The radius of gyration of individual chains also display as non-monotonic behavior which in part be explained by the scaling law in semi-dilute solutions, and with the increasing effective excluded due to adsorption of cosolvent. At higher attraction strengths a jump-like collapse of the polymer volume can be observed which corresponds to a type-II phase transition of the polymer solution. For interaction strengths greater than critical, two states of polymer solution coexists. Furthermore we have calculated the single-chain and collective structure factors. The dynamics was studied and the monomer diffusion coefficient was presented as a function of attraction strength.

CPP 22.23 Wed 16:30 CPPp

**Challenges and limits of Mechanical Stability in 3D Direct Laser Writing** — ●ELAHEH SEDGHAMIZ, MODAN LIU, and WOLFGANG WENZEL — Karlsruhe Institute of Technology, Karlsruhe, Germany

Direct laser writing is an effective technique for the fabrication of complex polymeric 3D polymer networks using ultrashort laser pulses. Practically, it remains a challenge to design and fabricate high-performance materials with different functions that possess a combination of high strength, substantial ductility, and tailored functionality, in particular for small feature sizes. To date, it is difficult to obtain a time-resolved microscopic picture of the printing process in operando. To close this gap, we have developed a molecular dynamics simulation approach to model direct laser writing and investigate the effect of writing condition and aspect ratio on the mechanical properties of the printed polymer network. We show that writing condition provides a possibility to tune the mechanical properties and an optimum writing condition can be applied to fabricate structures with improved mechanical properties. We reveal that beyond the writing parameters, aspect ratio plays an important role to tune the stiffness of the printed structures.

CPP 22.24 Wed 16:30 CPPp

**Periodic Boundary Calculations of photosensitive Ru(bpy)<sub>3</sub> complexes attached to polymer chains** — ●MIFTAHUSSURUR HAMIDI PUTRA and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany

Polymers are considered as potential candidate materials for the photocathodes of p-type dye sensitized solar cells (p-DSSCs), as they can be easily synthesized and are robust under operation conditions [1]. To optimize the performance of such solar cells, a better understanding of the structural and electronic coupling between the dyes and the polymer matrix is necessary which can be obtained through first-principles total energy calculations. However, dyes attached to polymer chains represent a challenge for quantum chemistry calculations because of their large system size. Here we present a first-principles computational study based on density functional theory of a Ru(bpy)<sub>3</sub> dye, one of the common dyes in p-DSSCs, attached to a polymer chain using a periodic boundary approach [2].

We will particularly address the geometrical and electronic coupling between the dye and the polymer chain and elucidate the changes in the optical properties of the dye upon the attachment to the polymer chain.

[1] Y. Pellegrin, L. Le Pleux, E. Blart, A. Renaud, B. Chavillon, N.

Szuwarski, M. Boujtita, L. Cario, S. Jobic, D. Jacquemin, and F. Odobel, *J. Photochem. Photobiol. A: Chem.* **219**, 235 (2011).  
 [2] A. Sen and A. Groß, *Int J Quantum Chem.* **119**, e25963 (2019).

CPP 22.25 Wed 16:30 CPPp

**Machine learning approach to long time step molecular dynamics for hard sphere systems** — •KA CHUN CHAN and WOLFGANG WENZEL — Institute of Nanotechnology Technology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen, Germany

Atomistic simulation techniques such as molecular dynamics (MD) provide an accurate and precise description of atomic motion, molecular structure and permit the prediction of the physical and chemical properties of molecular system. However, MD requires expensive computation of energy and force which leads to significant computational effort. This severely limits MD applications to biological system and soft matter physics on long time scales.

The usual MD time step is approximately 1/10 of the fastest frequency of the molecular system. In order to accelerate the MD computation, we propose a machine learning approach to propagate the molecular system instead of the usual MD time step. As a first step we developed a machine learning (ML) propagator for hard-sphere systems that propagates the molecular system with each atomic collision as a new time step. The proposed algorithm learns the time evolution of the atomic motion and the collision between atoms, such that the neural network are able to predict the system trajectory, identify the collided atomic pairs and correct the trajectory of the collided pairs for each collision time step. We will discuss the perspective of this newly ML propagator for the acceleration of MD simulations and further application to the molecular system with long time scales.

CPP 22.26 Wed 16:30 CPPp

**Kinetic Monte Carlo modeling of graphene growth on chemical vapor deposition.** — •MEYSAM ESMAELPOUR, MARIANA KOZLOWSKA, and WOLFGANG WENZEL — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Germany

Chemical vapor deposition (CVD) is the most promising method for high quality, large area graphene synthesis. Optimization of this chemical process will enable control over crucial properties, such as graphene quality and domain size. This requires the development of a detailed atomistic understanding of the underlying processes guiding the growth mechanism. In particular there is a need to understand the mechanism behind graphene nucleation and growth during CVD and its dependence on the synthetic parameters: temperature, CVD pressure, catalyst type, facet etc.

The complexity of CVD prohibits a complete description of all reaction mechanisms at the DFT level. Using the library of surface reaction rates, we have developed a Kinetic Monte Carlo (KMC) method to study the process of CVD of graphene from methane on Cu(111) under different synthesis conditions. It explains how synthesis parameters affect the quality and domains size of graphene. The results are compared with experimental measurements, enabling better understanding of the CVD mechanism.

CPP 22.27 Wed 16:30 CPPp

**A theoretical and computational study of ionic liquid mixtures in front of charged surfaces** — •TAKESHI KOBAYASHI, MARIA FYTA, and JENS SMIAŁEK — Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

The properties of the electric double layer formed in front of charged surfaces in room temperature ionic liquids (RTILs) solutions are studied by means of atomistic Molecular Dynamics simulations and the theory of the Lattice Boltzmann Gas model. We study 1-Ethyl-3-methylimidazolium dicyanamide ([EMIm]<sup>+</sup>[DCA]<sup>-</sup>) with water or dimethyl sulfoxide (DMSO) mixtures at different concentrations in order to investigate the solvent effects on the IL structuring in front of the surfaces. Our results reveal clear differences between water and DMSO mixtures at the interfaces. By applying the Lattice Boltzmann Gas model, the entropic and enthalpic contributions to the accumulation of the solvent molecules are discussed. The differences mainly appear in front of the positively charged interface where water accumulation but DMSO depletion occurs. Such outcomes are assigned to the combination of size and polarity of water or DMSO and the corresponding interactions with the cations or the anions in the solution. Overall, our results provide a deep understanding of the ionic liquid (IL) behavior close to interfaces and links to a proper selection of IL-

based mixtures in order to optimize specific technological applications.

CPP 22.28 Wed 16:30 CPPp

**A computational model for the study of catalysts in the Supported Ionic Liquid Phase in mesoporous media** — •TAKESHI KOBAYASHI<sup>1</sup>, HAMZEH KRAUS<sup>2</sup>, NIELS HANSEN<sup>2</sup>, and TAKESHI KOBAYASHI<sup>1</sup> — <sup>1</sup>Institute for Computational Physics, University of Stuttgart, Germany — <sup>2</sup>Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Germany

We set-up a model for the investigation of a linker-free immobilization of catalysts in confined media in an ionic liquid (IL)-mixture. Specifically, we study the mixture of n-heptane and 1-Butyl-3-methylimidazolium trifluoromethanesulfonate ([BMIm]<sup>+</sup>[Otf]<sup>-</sup>) in a closed pore geometry with a pore diameter of 5nm. The inner walls of the pore are functionalized in order to tune the polarity of the pore and its interaction with the solvent. The immobilization of the catalyst is expected to lead to higher turnover rates in the catalysis. Using Molecular Dynamics simulations, we model the catalyst in the IL-heptane mixture within the nanopore. Our simulations reveal that the IL accumulates within the pore, while we also follow the dynamics of all molecules involved in the system. Using quantum mechanical calculations, we parameterize a force-field for the catalyst, which is being further used for a more accurate model of the catalyst within the IL-mixture. Our results provide important information on the influence of steric and IL-specific effects, the structuring of a varying solvent environment, the pore functionality, and their interactions with the catalytic center. These aspects promote a rational design of the catalyst immobilization and point to the relevant conditions.

CPP 22.29 Wed 16:30 CPPp

**Self-assembly of silica nanoparticles guided by directional crystallization of grafted polymers** — •ASWATHY MUTTATHUKATIL<sup>1</sup>, AFSHIN NABIYAN<sup>2</sup>, FEDERICO TOMAZIC<sup>1</sup>, FELIX HELMUT SCHACHER<sup>2</sup>, and MICHAEL ENGEL<sup>1</sup> — <sup>1</sup>Institute for Multiscale Simulation, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 3, 91058 Erlangen, Germany — <sup>2</sup>Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich-Schiller University Jena, Lessingstraße 8, 07743 Jena, Germany

Self-assembly of nanoparticles (NP) is an efficient bottom-up approach to produce nanostructures with complex architectures. Here, we report the formation of an inorganic-organic hybrid network by self-assembly of silica NPs grafted by poly(2-iso-propyl-2-oxazoline)(PIPOX) at elevated temperatures. To resolve the underlying molecular mechanism, we utilize coarse-grained molecular dynamics simulations. Earlier reports stated that PIPOX polymers crystallize into long fibers guided by directional dipolar interactions between amide groups. Building on this information, we represent PIPOX monomers by spherical, patchy beads. Chains of patchy beads represent polymer is attached to NP sphere. Our simulations of this NP-polymer system characterize the two steps of the self-assembly process: (1) rapid formation of amorphous aggregates via gelation, mediated by interaction between NPs through grafted polymers; (2) slower formation of diverging fibers via directional crystallization of unbound polymers with the grafted polymer matrix. The understanding of the molecular mechanism is a step towards targeted self-assembly for catalysis and other applications.

CPP 22.30 Wed 16:30 CPPp

**Low-symmetry phases in attraction-driven assembly of nanotriangles** — •MARCO KLEMENT and MICHAEL ENGEL — Institute for Multiscale Simulation, IZNF, FAU Erlangen, Erlangen, Germany

Hard triangles at high packing density spontaneously order into high-symmetry phases [1,2] with wallpaper groups p6 and p6mm. Recent experiments with coated nanotriangles [3] observed additional phases with wall paper groups pmg and p2. The appearance of these low-symmetry phases depends on the contour length and grafting density of surfactant polymer ligand molecules. We develop a novel simulation algorithm for anisotropic interacting nanoparticles, which attribute a majority of the observations to effective rounding of triangle vertices. The remaining observation, a p2 symmetric phase for the shortest molecules in use is a consequence of a soft attractive interaction of surfactant molecules.

[1] Gantapara, A. P., Qi, W., and Dijkstra, M. "A novel chiral phase of achiral hard triangles and an entropy-driven demixing of enantiomers". *Soft Matter* **11**, 8684-8691 (2015).

[2] Walker, D. A., Browne, K. P., Kowalczyk, B., and Grzybowski, B. A. "Self-Assembly of Nanotriangle Superlattices Facilitated by Repulsive Electrostatic Interactions." *Angewandte Chemie International*

Edition 49, 6760\*6763 (2010).

[3] Liu, Yang and Klement, Marco and Zhong, Yaxu and Chen, Jun and Engel, Michael and Ye, Xingchen, "Using Ligand Engineering to Control Self-Assembly of Polyesterol Coated Nano Triangles", in preparation (2021)

CPP 22.31 Wed 16:30 CPPp

**Pendant drop tensiometry: A machine learning approach** — ●FELIX KRATZ and JAN KIERFELD — Department of Physics, TU Dortmund University, Dortmund, Germany

Modern pendant drop tensiometry relies on the numerical solution of the Young-Laplace equation and allows us to determine the surface tension from a single picture of a pendant drop with high precision. Most of these techniques solve the Young-Laplace equation many times over to find the material parameters that provide a fit to a supplied image of a real droplet. Here, we introduce a machine learning approach to solve this problem in a computationally more efficient way. We train a deep neural network to determine the surface tension of a given droplet shape using a large training set of numerically generated droplet shapes. We show that the deep learning approach is superior to the current state of the art shape fitting approach in speed and precision, in particular if shapes in the training set reflect the sensitivity of the droplet shape with respect to surface tension. In order to derive such an optimized training set, we clarify the role of the Worthington number as a quality indicator in conventional shape fitting and in the machine learning approach. Our approach demonstrates the capabilities of deep neural networks in the material parameter determination from rheological deformation experiments, in general.

CPP 22.32 Wed 16:30 CPPp

**Magneto-mechanical response of nanoscale magnetic filaments** — DENIZ MOSTARAC<sup>1</sup>, PEDRO A. SÁNCHEZ<sup>1,2</sup>, and ●SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>University of Vienna, Vienna, Austria. — <sup>2</sup>Ural Federal University, Ekaterinburg, Russia.

Nanoscale magnetic filaments (MFs) are magnetic, nano-sized colloids, crosslinked into polymer-like linear chains. They are a promising platform for engineering new magnetically controlled filtering and flow control elements in micro-fluidic devices. Recent advances, advocating an assembly mechanism where the structure building instructions are embedded into nanoparticles via DNA origami frames, synthesis of MFs with desirable mechanical properties.[2,3] Using MD simulations we have studied how possible crosslinking scenarios and magnetic nature of monomers (ferromagnetic or super-paramagnetic) influence equilibrium properties of MFs.[4] In this contribution, we elucidate an interesting phenomenology of MFs, by examining their behaviour in a Langevin thermostat (equilibrium properties) and explicit solvent representations using the Lattice Boltzmann method (dynamics in rotating magnetic fields). Magnetization of super-paramagnetic monomers is taken into account in an accurate manner, inclusive of non-linear contributions. [1] Sánchez, P. A., et al. *Macromolecules* 48.20 (2015): 7658-7669. [2] Liu, W., et al. *Nature chemistry* 8.9 (2016): 867. [3] Tian, Y., et al. *Nature materials* 15.6 (2016): 654. [4] Mostarac, D., et al. *Nanoscale* (2020).

CPP 22.33 Wed 16:30 CPPp

**Directing the Diffusion of a Nonmagnetic Nanosized Active Particle with External Magnetic Fields** — ●MARTIN KAISER<sup>1</sup> and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — <sup>2</sup>Ural Federal University, Lenin Av. 51, Ekaterinburg 620000, Russian Federation

With the help of molecular dynamics simulations we show that an arbitrary non-magnetic active particle with a size below one micrometer, being immersed in a polydisperse system of magnetic nanoparticles, can diffuse twice faster along the direction of the applied field than perpendicular to the latter, whereas, for a monodisperse system, the ratio between diffusion coefficients parallel and perpendicular to the field approaches two orders of magnitude, even for magnetic fields of moderate strength. The ability to direct a non-magnetic active particle along the magnetic field stems from the formation of chains of magnetic nanoparticles aligned with the field direction. Such chains form effective channels through which the active particle can diffuse. We find that the ability to direct an active particle of a given size can be maximised by changing magnetic particle concentration so that the tunnels formed by the change have a mean width of approximately the active particle size.

CPP 22.34 Wed 16:30 CPPp

**Deformation of Azo-Polymer Droplets by Light: Modeling the Effects of Light on Glassy Azobenzene Materials** — ●MARKUS KOCH, MARINA SAPHIANNIKOVA, and OLGA GUSKOVA — Institute Theory of Polymers, IPF Dresden, Germany

Azobenzene (azo) is the most widespread light-responsive molecule due to its well-studied trans-cis photoisomerization mechanism. This compound has gained prominence due to the possibility to create surface relief gratings in azo-polymer materials using light interference patterns. However, it remains an open question how light induces mechanical stresses in the material. To study this process we consider a model system: A droplet composed of PMMA with azobenzene side chains is exposed to linearly polarized UV-Vis light. Experiments demonstrate, that such droplets deform along the polarization direction [1]. Here, using all-atom MD simulations two different approaches are applied: In the first case, the angle-dependent photoisomerization of azobenzene is simulated explicitly. In the second case, an effective orientation potential acts on the azo groups [2]. We demonstrate that both approaches lead to the reorientation of azobenzene in the polymer matrix and discuss the induced deformation of the droplet.

We thank the German Research Foundation (DFG) for financial support, project GU 1510/5-1.

[1] Loebner, S. et al., *J. Phys. Chem. B*, 122 (6), 2001-2009 (2018)

[2] Toshchevnikov, V. et al. *J. Phys. Chem. Lett.*, 8 (5), 1094-1098 (2017)

CPP 22.35 Wed 16:30 CPPp

**End-Adsorbing Chains in Polymer Brushes: Pathway to Highly Metastable Switchable Surfaces** — ●MARKUS KOCH<sup>1</sup>, DIRK ROMEIS<sup>1</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Institute Theory of Polymers, IPF Dresden, Germany — <sup>2</sup>Institute Theory of Physics, TU Dresden, Germany

Polymer brushes are promising systems for the design of stimulus-responsive surfaces. In addition, it is often highly desirable to controllably hide or expose functional groups. To this end, we investigate monodisperse polymer brushes, which contain a small fraction of end-modified minority chains [1]. The length of these chains is variable and their end groups can adsorb to the grafting surface. We study these systems using Scheutjens-Fleer SCF calculations [2], MD simulations, and analytical theory. The conformational changes of the admixed chains are explored, which depend on their length and the attraction between their end groups and the surface. Based on the free energy profiles of the adsorption transition, free energy barriers are extracted, which are in good agreement with our theoretical predictions. The barriers are strongly reduced upon the collapse of the brush and can be tuned to attain reversible or irreversible switching 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 (2021)

[2] Fleer, G. J., et al. *Polymers at Interfaces*. London, Chapman and Hall, 1993

CPP 22.36 Wed 16:30 CPPp

**Fast high-accuracy optimization of delocalized Gaussian sets for eigenfunctions** — MOHAMMADREZA EIDI, ●BENJAMIN RABE, and JAN-MICHAEL ROST — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Gaussian basis sets are widely used to represent the wave function of atomic and molecular systems due to their great advantage that matrix elements with Gaussians at different locations can often be calculated analytically [1]. However, it is not trivial to optimize for a large set of Gaussians  $\{exp(-\alpha_i(x-x_i)^2) | i = 1, \dots, N\}$  the parameters  $\{\alpha_i, x_i\}$ . Procedures with predefined positions following a geometric series, so called even tempered basis sets (e.g. [2]), have been put forward. Here we introduce an iterative scheme which optimizes positions and widths simultaneously for a given number  $N$  of s-type Gaussians. To this end we use only during the optimization process auxiliary Gaussians which have in 3D angular momentum p and d character. This way one gets highly accurate results at low computational cost, even for small numbers of Gaussians. We will demonstrate how the method works with explicit 1D examples for various potentials representing atomic and molecular scenarios. [1] Mitroy, Jim, et al., *Rev. Mod. Phys.* 85.2 (2013): 693. [2] Cherkes, I., Klaiman, S., and Moiseyev, N., *Int. J. Quantum Chem.* 109, 2996 (2009).

CPP 22.37 Wed 16:30 CPPp

**Phase behavior of polymeric microemulsion in ternary**

**A+B+AB blends** — ●RUSSELL SPENCER<sup>1</sup> and MARK MATSEN<sup>2</sup> — <sup>1</sup>Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — <sup>2</sup>Department of Chemical Engineering, Department of Physics & Astronomy, and Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada

Ternary blends of AB diblock copolymers with A and B homopolymers microphase segregate into lamellae (LAM) for copolymer-rich blends and macrophase segregate into A- and B-rich regions for homopolymer-rich blends. Mean-field theory predicts that these regions are separated by three-phase coexistence of the LAM, A-rich, and B-rich phases, which terminates at a Lifshitz critical point. Experiments, however, report that the Lifshitz point is destroyed by fluctuations and that the three-phase coexistence is replaced by a channel of bicontinuous microemulsion (B $\mu$ E). Using field-theoretic simulations, we show that fluctuations do indeed destroy the Lifshitz point, but that three-phase coexistence continues to exist. However, at high temperatures, the LAM+A+B coexistence predicted by mean-field theory is replaced by B $\mu$ E+A+B coexistence. We speculate that the single-phase B $\mu$ E observed in experiments is a result of kinetic trapping as the blend is cooled from the mixed state.

CPP 22.38 Wed 16:30 CPPp

**Understanding the static and dynamic behaviour of stars forming reversible networks** — ●KIRAN SURESH KUMAR<sup>1,2</sup>, TONI MÜLLER<sup>1,2</sup>, JENS-UWE SOMMER<sup>1,2</sup>, and MICHAEL LANG<sup>1</sup> — <sup>1</sup>Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — <sup>2</sup>Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Reversible networks break and reform continuously allowing the material to flow and self-heal on long time scales while being a solid on short times. Recent experiments and simulation studies find an apparent anomalous superdiffusive regime in reversible networks by analyzing Forced Rayleigh Scattering (FRS) data [1-3]. The molecular origin of this superdiffusive regime is not yet fully understood. In our contribution, we approach this problem by computer simulations of FRS experiments in reversible networks using the Bond Fluctuation Model. We analyze the static properties and the connectivity of individual stars and develop an analytic model for the statistics of connections. We analyze dynamic properties of individual stars and compute the collective relaxation as accessible in FRS. Our goal is to develop a model based upon the molecular statistics that allows to quantitatively predict the collective dynamics of the reversible network.

[1] Tang, S.; Wang, M.; Olsen, B. D. *J. Am. Chem. Soc.* 2015, 137, 3946-3957. [2] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. *Macromolecules* 2016, 49, 5599-5608. [3] Ramirez, J.; Dursch, T. J.; Olsen, B. D. *Macromolecules* 2018, 51, 2517-2525.

CPP 22.39 Wed 16:30 CPPp

**Self-Assembly of Copolymers in Presence of Solvent Evaporation** — ●GREGOR IBBEKEN and MARCUS MÜLLER — Institut für Theoretische Physik, Georg August Universität, Friedrich-Hund-Platz 1, 37077 Göttingen, Deutschland

Integral asymmetric block copolymer membranes constitute a fascinating new technology for ultrafiltration. Solvent evaporation aligns and facilitates the long-range order of microphase separating diblock copolymers, which is exploited to form monodisperse pores. More specifically, we are interested in the emergence of perpendicularly oriented, cylindrical morphologies. We investigate a system consisting of a diblock copolymer, a solvent and air by use of a continuum model in which the concentrations act as order parameters. This allows us to explore the high-dimensional parameter space with a parameter study. Four parameters turn out to have a dominant influence on emergent morphologies, namely the polymer volume fraction, the surface preference, the incompatibility of polymer blocks and the evaporation rate. Kinetically, the orientation of cylinders is determined immediately after the onset of microphase separation. If cylinders become stable when the evolution zone is wide enough, initially developed spheres elongate vertically. Most notably, this occurs for high evaporation rates. Additionally, we are able to demonstrate that the kinetic pathways taken are describable as paths in a two-dimensional parameter space consisting of effective block ratio  $f^{eff}$  and effective segregation strength  $\chi N_{ab}^{eff}$ .

CPP 22.40 Wed 16:30 CPPp

**Magnetic nanogels in magnetic field** — ●IVAN NOVKAU<sup>1</sup>, PEDRO

SANCHEZ<sup>1</sup>, and SOFIA KANTOROVICH<sup>1,2</sup> — <sup>1</sup>University of Vienna — <sup>2</sup>Ural Federal University

Nanogels (NGs) with multifunctionalized magnetic nanoparticles (MNPs) have demonstrated the ability to effectively destroy cancer cells *in vivo*, without causing visible damage to healthy organs [1]. The presence of MNPs inside the NGs also offers an additional mechanism to control their properties by means of applied magnetic fields.

Our study of a suspension of NGs loaded with MNPs in zero-field case showed that the structural properties of a single gel, and the self-assembly in the given system, strongly depend on the strength of the dipole-dipole interaction (dipolar coupling parameter) between the MNPs [2].

Here, we investigate a suspension of magnetic NGs in a constant external magnetic field by means of molecular dynamics computer simulations [3]. Each NG is initially modeled as a system of bead-spring polymer chains randomly cross-linked into a polymer network. MNPs are arbitrary incorporated into this network.

We find that even weak fields lead to drastic changes in the structure factors of both, the embedded MNPs and of whole NGs. But what is even more curious, is that the polymer matrix of nanogels enhances the magnetization of free MNPs.

[1] Qing Wu et al., *Nat. Commun.*, 10 (240), 2019.

[2] Novikau et al., *JMMM*, 498, 2020.

[3] Novikau et al., *J. Mol. Liq.*, 307, 2020.

CPP 22.41 Wed 16:30 CPPp

**Water purification with pvdf membrane** — ●RENÉ HAFNER<sup>1,2</sup> and PETER KLEIN<sup>1</sup> — <sup>1</sup>Fraunhofer ITWM, Kaiserslautern, Deutschland — <sup>2</sup>TUK, Kaiserslautern, Deutschland

We investigate the interaction of crystal and amorphous Polyvinylidenfluorid (PVDF) membranes with the pharmaceutical diclofenac, i.e. an inflammatory pain killer, as a surrogate of a wider class of charged drug molecules via the potential of mean force (PMF) method. While the crystal membrane is in polar beta zigzag form of PVDF, both are created by a structure generator of our own. We further highlight the features of our structure generator. For both membrane and diclofenac the Charmm force field is used. Simulations were conducted using the simulation software NAMD. The PMFs between drug and membrane are obtained via the adaptive biasing force method ABF and its extended version. Comparison is drawn between amorphous and crystal PVDF membranes and their adsorption capabilities are discussed.

CPP 22.42 Wed 16:30 CPPp

**Separable intermolecular force fields from first principles** — ●MANUEL KONRAD and WOLFGANG WENZEL — Institute of Nanotechnology, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

The decomposition of intermolecular interactions into physically meaningful components can be a useful tool to gain a deeper understanding about non-covalently bonded complexes. However, separable *ab initio* methods, such as symmetry adapted perturbation theory (SAPT), are limited to small systems. Here we present a systematic approach to derive an analytical force field from a finite number of SAPT calculations while preserving the energy decomposition of the reference method. For several small organic molecules, we apply this model in molecular dynamics simulations to compute thermodynamic properties. The comparison against experimental values shows promising prediction capabilities. Together with the additional insight from the energy decomposition, this makes our method a potentially versatile tool for the *in silico* discovery of new molecular materials, where force field parametrizations can't rely on experimental target data.

CPP 22.43 Wed 16:30 CPPp

**Structure formation in 2D-Copolymer Networks** — ●GAOYUAN WANG and MARCUS MÜLLER — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

Two-dimensional polymer networks, characterized by a planar geometry, open new possibilities for the design of polymer molecules with novel properties. Using large-scale simulations, we study microphase separation in two-dimensional, defect-free, interpenetrating phantom networks, obtained by crosslinking symmetric diblock copolymers. The system exhibits a complex interplay between the network structure, characterized by the length (geometry) of a unit cell, and the lamellar microphase with its periodicity that depends on the incompatibility between the blocks. We investigate the incompatibility at which system microphase separates as a function of the size of the (unper-

turbed) unit cell of the network and quantify the network structure in the microphase-separated state. Our findings are compared to the mi-

crophase separation linear diblock, triblock and multiblock copolymers as well as to the mechanical properties of networks.