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Fachverband Chemische Physik und Polymerphysik (CPP)

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Overview of Invited Talks and Sessions
(Lecture halls H1 and H3; Poster P)

Invited Talks

CPP 2.1	Mon	13:30–14:00	H1	**On the permeability of dense polymer membranes** — •Joachim Dzubiella
CPP 3.1	Mon	13:30–14:00	H3	**Emulsion Templating: Unexpected Morphology of Monodisperse Macroporous Polystyrene** — •Cosima Stubenrauch, Lukas Koch, Sophia Botsch, Wiebke Drenckhan
CPP 3.4	Mon	14:30–15:00	H3	**Structural Transitions of Molecules on Surfaces** — •Angelika Kühnle
CPP 4.1	Tue	10:00–10:30	H3	**Adaptable amphiphilic co-networks: structure and properties in relation with multi-quantum NMR** — •Michael Lang, Reinhard Scholz, Lucas Löser, Carolin Bunk, Frank Böhme, Kay Saalwächter
CPP 4.2	Tue	10:30–11:00	H3	**Adaptive networks through supramolecular interactions** — •Ilja Voets
CPP 4.5	Tue	11:45–12:15	H3	**Tunable self-assembled hydrogels from block copolymers with thermoresponsive and pH-responsive blocks** — •Christine M. Papadakis, Florian A. Jung, Constantinos Tsitsilianis
CPP 7.1	Wed	10:00–10:30	H3	**Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems** — •Andreas Walther
CPP 7.4	Wed	11:15–11:45	H3	**The quest for robust superhydrophobic surfaces** — •Robin Ras
CPP 10.1	Thu	13:30–14:00	H3	**Nanophotonic structures by inkjet printing** — Yidenekachew J. Donie, Qiaoshuang Zhang, Guillaume Gomard, •Uli Lemmer
CPP 13.1	Fri	10:00–10:30	H3	**Electron-lattice relaxation effects in halide perovskites** — •David A. Egger
CPP 13.6	Fri	11:45–12:15	H3	**Light-actuated colloidal nano- and microparticles** — •Cornelia Denz, Matthias Rueschenbaum, Valeria Bobkova, Julian Jeggle, Raphael Wittkowski
CPP 15.1	Fri	13:30–14:00	H3	**Data-driven protein design and simulation** — •Andrew Ferguson

Invited talks of the joint symposium Topological constraints in biological and synthetic soft matter (SYSM)
See SYSM for the full program of the symposium.

SYSM 1.1	Mon	10:00–10:30	Audimax 1	**Interphase Chromatin Undergoes a Local Sol-Gel Transition Upon Cell Differentiation** — •Alexandra Zidovska
SYSM 1.2	Mon	10:30–11:00	Audimax 1	**Topological Tuning of DNA Mobility in Entangled Solutions of Supercoiled Plasmids** — •Jan Smrek, Jonathan Garamella, Rae Robertson-Anderson, Davide Michieletto
SYSM 1.3	Mon	11:15–11:45	Audimax 1	**Dynamics of macromolecular networks under topological and environmental constraints: some outstanding challenges** — •Dimitris Vlassopoulos
SYSM 1.4	Mon	11:45–12:15	Audimax 1	**Supercoiling in a Protein Increases its Stability** — •Joanna Sulkowska, Szymon Niewieczerzał
SYSM 1.5	Mon	12:15–12:45	Audimax 1	**Topology for soft matter photonics** — •Igor Musevic

Invited talks of the joint symposium SKM Dissertation Prize 2021 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:00–10:25	Audimax 2	**Avoided quasiparticle decay from strong quantum interactions** — •Ruben Verresen, Roderich Moessner, Frank Pollmann
SYSD 1.2	Mon	10:25–10:50	Audimax 2	**Co-evaporated Hybrid Metal-Halide Perovskite Thin-Films for Optoelectronic Applications** — •Juliane Borchert
SYSD 1.3	Mon	10:55–11:20	Audimax 2	**Attosecond-fast electron dynamics in graphene and graphene-based interfaces** — •Christian Heide
SYSD 1.4	Mon	11:20–11:45	Audimax 2	**The thermodynamics of stochastic systems with time delay** — •Sarah A.M. Loos
SYSD 1.5	Mon	11:50–12:15	Audimax 2	**First Results on Atomically Resolved Spin-Wave Spectroscopy by TEM** — •Benjamin Zingsem

Invited talks of the joint symposium Multidimensional coherent spectroscopy of functional nanostructures (SYCS)

See SYCS for the full program of the symposium.

SYCS 1.1	Tue	10:00–10:30	Audimax 1	**Multidimensional coherent spectroscopy of perovskite nanocrystals** — •Steven Cundiff, Albert Liu, Diogo Almeida, Gabriel Nagamine, Lazaro Padilha
SYCS 1.2	Tue	10:30–11:00	Audimax 1	**Coherent multidimensional techniques for the characterization of nanomaterials** — •Elisabetta Collini
SYCS 1.3	Tue	11:00–11:30	Audimax 1	**Exciton Dynamics revealed by Multidimensional Coherent Spectroscopies applied to Light-Harvesting Systems** — •Thomas L.C. Jansen
SYCS 1.4	Tue	11:45–12:15	Audimax 1	**Revealing couplings with action-based 2D microscopy** — •Tobias Brixner
SYCS 1.5	Tue	12:15–12:45	Audimax 1	**Low-frequency phonons affect charge carrier dynamics in hybrid perovskites** — •Mischa Bonn

Invited talks of the joint symposium Amorphous materials: structure, dynamics, properties (SYAM)

See SYAM for the full program of the symposium.

SYAM 1.1	Tue	13:30–14:00	Audimax 1	**Glassy dynamics of vitrimers** — •Liesbeth Janssen
SYAM 1.2	Tue	14:00–14:30	Audimax 1	**Liquid-Liquid Phase Transition in Thin Vapor-Deposited Glass Films** — •Zahra Fakhraai
SYAM 1.3	Tue	14:30–15:00	Audimax 1	**Connection between structural properties and atomic motion in ultraviscous metallic liquids close to the dynamical arrest** — •Beatrice Ruta, Nico Neuber, Isabella Gallino, Ralf Busch
SYAM 1.4	Tue	15:15–15:45	Audimax 1	**Signatures of the spatial extent of plastic events in the yielding transition in amorphous solids** — •Celine Ruscher, Daniel Korchinski, Joerg Rottler
SYAM 1.5	Tue	15:45–16:15	Audimax 1	**Constitutive law for dense agitated granular flows: from theoretical description to rheology experiment** — •Olfa D'Angelo, W. Till Kranz

Invited talks of the joint symposium Curvilinear condensed matter (SYCL)

See SYCL for the full program of the symposium.

SYCL 1.1	Wed	10:00–10:30	Audimax 2	**Curvature Effects and Topological Defects in Chiral Condensed and Soft Matter** — •Avadh Saxena
SYCL 1.2	Wed	10:30–11:00	Audimax 2	**Topology and Transport in nanostructures with curved geometries** — •Carmine Ortix
SYCL 2.1	Wed	11:15–11:45	Audimax 2	**Superconductors and nanomagnets evolve into 3D** — •Oleksandr Dobrovolskiy
SYCL 2.2	Wed	11:45–12:15	Audimax 2	**Properties of domain walls and skyrmions in curved ferromagnets** — •Volodymyr Kravchuk

SYCL 2.3   Wed   12:15–12:45   Audimax 2   **X-ray three-dimensional magnetic imaging** — •Valerio Scagnoli

Prize talks of the joint Awards Symposium (SYAW)
See SYAW for the full program of the symposium.

SYAW 1.1	Wed	13:30–14:00	Audimax 1	**Organic semiconductors - materials for today and tomorrow** — •Anna Köhler
SYAW 1.2	Wed	14:00–14:30	Audimax 1	**PbTe/CdTe nanocomposite as an attractive candidate for room-temperature infrared detectors** — •Grzegorz Karczewski
SYAW 1.3	Wed	14:40–15:10	Audimax 1	**Fingerprints of correlation in electronic spectra of materials** — •Lucia Reining
SYAW 1.4	Wed	15:10–15:40	Audimax 1	**Artificial Spin Ice: From Correlations to Computation** — •Naëmi Leo
SYAW 1.5	Wed	15:40–16:10	Audimax 1	**From microwave optomechanics to quantum transport – carbon nanotubes as highly versatile hybrid devices** — •Andreas K. Hüttel
SYAW 1.6	Wed	16:20–16:50	Audimax 1	**Quantum spin dynamics of a spin-$1/2$ antiferromagnetic Heisenberg-Ising chain** — •Zhe Wang
SYAW 1.7	Wed	16:50–17:20	Audimax 1	**Imaging the effect of electron transfer at the atomic scale** — •Laerte Patera

Invited talks of the joint symposium Spain as Guest of Honor (SYES)
See SYES for the full program of the symposium.

SYES 1.1	Wed	13:30–13:40	Audimax 2	**DFMC-GEFES** — •Julia Herrero-Albillos
SYES 1.2	Wed	13:40–14:10	Audimax 2	**Towards Phononic Circuits based on Optomechanics** — •Clivia M. Sotomayor Torres
SYES 1.3	Wed	14:10–14:40	Audimax 2	**Adding magnetic functionalities to epitaxial graphene** — •Rodolfo Miranda
SYES 1.4	Wed	14:45–15:15	Audimax 2	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 1.5	Wed	15:15–15:45	Audimax 2	**Hydrodynamics of collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.6	Wed	15:45–16:15	Audimax 2	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs

Invited talks of the joint symposium Diversity on the Device Scale (SYHN)
See SYHN for the full program of the symposium.

SYHN 1.1	Thu	10:00–10:30	Audimax 1	**Scaling behavior of stiffness and strength of hierarchical network nanomaterials** — •Shan Shi
SYHN 1.2	Thu	10:30–11:00	Audimax 1	**Functional and programmable DNA nanotechnology** — •Laura Na Liu
SYHN 1.3	Thu	11:15–11:45	Audimax 1	**Multivalent nanoparticles for targeted binding** — •Stefano Angioletti-Uberti
SYHN 1.4	Thu	11:45–12:15	Audimax 1	**Programming Nanoscale Self-Assembly** — •Oleg Gang
SYHN 1.5	Thu	12:15–12:45	Audimax 1	**Achieving Global Tunability via Local Programming of a Structure's Composition** — •Jochen Mueller

Invited talks of the joint symposium Active nematics: From 2D to 3D (SYAN)
See SYAN for the full program of the symposium.

SYAN 1.1	Fri	10:00–10:30	Audimax 1	**Corrugated patterns made from an active nematic sheet** — •Anis Senoussi, Shunichi Kashida, Raphaël Voituriez, Jean-Christophe Galas, Ananyo Maitra, Estevez-Torres André
SYAN 1.2	Fri	10:30–11:00	Audimax 1	**Wrinkling instability in 3D active nematics** — •Isabella Guido
SYAN 1.3	Fri	11:15–11:45	Audimax 1	**Three-dimensional active nematic defects and their energetics** — •Miha Ravnik

SYAN 1.4	Fri	11:45–12:15	Audimax 1	**Liquid-crystal organization of liver tissue** — •Benjamin M Friedrich, Hernan Morales-Navarrete, Andre Scholich, Hidenori Nonaka, Fabian Segovia Miranda, Steffen Lange, Jens Karschau, Yannis Kalaidzidis, Frank Jülicher, Marino Zerial
SYAN 1.5	Fri	12:15–12:45	Audimax 1	**Machine learning active nematic hydrodynamics** — •Vincenzo Vitelli

Sessions

CPP 1.1–1.7	Mon	11:15–13:00	H3	**2D materials and their heterostructures (joint session DS/HL/CPP)**
CPP 2.1–2.3	Mon	13:30–14:30	H1	**Hydrogels and Microgels**
CPP 3.1–3.8	Mon	13:30–16:15	H3	**Polymer Physics**
CPP 4.1–4.7	Tue	10:00–12:45	H3	**Focus: The Physics of Adaptive Polymer Networks**
CPP 5.1–5.19	Tue	17:30–19:30	P	**Poster Session I**
CPP 6.1–6.26	Tue	17:30–19:30	P	**Poster Session II**
CPP 7.1–7.8	Wed	10:00–12:45	H3	**Soft Matter (joint session CPP/DY)**
CPP 8.1–8.32	Wed	17:30–19:30	P	**Poster Session III**
CPP 9.1–9.5	Thu	11:45–13:00	H2	**Active Matter (joint session DY/BP/CPP)**
CPP 10.1–10.9	Thu	13:30–16:15	H3	**Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)**
CPP 11.1–11.4	Thu	15:15–16:15	H5	**Thin Oxides and Organic Thin Films (joint session DS/CPP)**
CPP 12	Thu	17:30–18:30	MVCPP	**Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)**
CPP 13.1–13.8	Fri	10:00–12:45	H3	**Molecular Electronics, Hybrid and Perovskite Photovoltaics**
CPP 14.1–14.4	Fri	10:00–11:00	H2	**Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)**
CPP 15.1–15.5	Fri	13:30–15:00	H3	**Theory and Simulation (joint session CPP/DY)**

Annual General Meeting of the Chemical and Polymer Physics Division

Thursday   17:30–18:30   MVCPP

- Report of the current speaker team
- Election of the second deputy speaker
- Miscellaneous

CPP 1: 2D materials and their heterostructures (joint session DS/HL/CPP)

Time: Monday 11:15–13:00

Location: H3

CPP 1.1   Mon 11:15   H3

Tunable phases of Moire excitons in van der Waals heterostructures — ●Samuel Brem[1], Christopher Linderälv[2], Paul Erhart[2], and Ermin Malic[1,2] — [1]Philipps University, Marburg, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

Two monolayers of Transition Metal Dichalogenides can be vertically stacked to form a type-II heterostructure, hosting spatially indirect interlayer excitons. Recent studies have shown that moire superlattices can be created by stacking monolayers with a finite twist-angle, giving rise to a tunable modification of exciton features in optical spectra. The moire patterns lead to a spatially varying band gap and consequently, excitons experience a periodic potential modifying their transport properties.

We have combined first-principles calculations with the excitonic density matrix formalism to develop an exciton model for small-angle twisted MoSe2/WSe2 heterostructures. Based on a microscopic approach, we calculate the band structure and wave functions of intra- and interlayer excitons within a twist-tunable moire lattice as well as the resulting optical response. For a range of small twist-angles, we predict completely flat exciton bands corresponding to moire trapped, localized quantum emitters. However, we reveal that this moire exciton phase quickly changes with increasing twist-angle, and at 3°, there are only delocalized excitons. We find the emergence of multiple moire exciton peaks in the absorption, whose spectral shifts with varying twist-angle are characteristic for the trapped or delocalized phase.

CPP 1.2   Mon 11:30   H3

Electrical control of spin-orbit coupling-induced spin precession and spin-to-charge conversion in graphene proximitized by WSe2 — ●Franz Herling[1], Josep Ingla-Aynes[1], C. K. Safeer[1], Nerea Ontoso[1], Jaroslav Fabian[2], Luis E. Hueso[1,3], and Felix Casanova[1,3] — [1]CIC nanoGUNE BRTA, Spain — [2]University of Regensburg, Germany — [3]IKERBASQUE, Basque Foundation for Science, Spain

When combined with WSe2, a large spin-orbit coupling gets imprinted by proximity effect into graphene. Here, we use this effect to achieve the strong SOC regime in bilayer graphene. Together with the long, gate tunable spin diffusion, this provides unique control knobs to manipulate coherent spin precession in the absence of an external magnetic field. Remarkably, we observe in these devices that the sign of the precessing spin polarization can be tuned electrically by a back gate voltage and by a drift current. This realization of a spin field-effect transistor at room temperature in a diffusive system, a long-awaited goal of spintronics, could be a cornerstone for the implementation of energy efficient spin-based logic.

In accordance with the large proximity-induced SOC, we also observe spin Hall effect in similar heterostructures with an unprecedented spin-to-charge conversion length of up to 41 nm. Such highly efficient conversion up to room temperature will play a crucial role for the future integration of spintronic devices into existing electronic infrastructure.

CPP 1.3   Mon 11:45   H3

Gate-Switchable Arrays of Quantum Light Emitters in Contacted Monolayer MoS₂ van der Waals Heterodevices — ●Alexander Hötger[1,2], Julian Klein[1,2,3,4], Katja Barthelmi[1,3], Lukas Sigl[1,2], Samuel Gyger[5], Takashi Taniguchi[6], Kenji Watanabe[6], Val Zwiller[5], Klaus D. Jöns[5], Ursula Wurstbauer[2,7], Jonathan Finley[1,2,3], and Alexander Holleitner[1,2,3] — [1]Walter Schottky Institut, TU Munich — [2]Exzellenzcluster e-conversion — [3]Munich Center for Quantum Science and Technology — [4]Massachusetts Institute of Technology, Cambridge — [5]KTH Royal Institute of Technology, Dept. of Applied Physics — [6]National Institute for Materials Science, Tsukuba — [7]Institute of Physics, Westfälische Wilhelms-Universität Münster

Controlling single-photon emission on a few nanometers plays an important role for the scalability of future quantum photonic circuits. Moreover, it is highly relevant to facilitate a gate-switchable emission for quantum information schemes. By irradiating MoS₂ with helium ions, we generate single-photon sources at ~1.75 eV with a lateral position accuracy of only a few nanometers. [1] Second-order correlation measurements unambiguously proof the nature of single-photon emis-

sion. Charge doping of the monolayer MoS₂ can be used for switching the quantum emission on and off. [2] This deterministic control of light emission in spatial and temporal means paves the way for new integrated quantum photonic technologies.

[1] J. Klein, L. Sigl et al., ACS Photonics 8, 2 (2021).
[2] A. Hötger et al., Nano Lett. 21, 2 (2021).

CPP 1.4   Mon 12:00   H3

Tunnelling transport in bilayer graphene nanostructures with quantum dots — ●Angelika Knothe[1], Vladimir Fal'ko[1], and Leonid Glazman[2] — [1]National Graphene Institute, University of Manchester, Manchester M13 9PL, United Kingdom — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, e.g., transistors or qubits. In gapped bilayer graphene (BLG), one can confine charge carriers electrostatically, inducing smooth confinement potentials while allowing gate-defined control of the confined structure. I will discuss charge transport in BLG nanostructures with electrostatically confined quantum dots. We investigate both theoretically and in collaboration with experiments how the BLG dots' highly degenerate single- and two-electron spin and valley multiplets, which depend on, e.g., the displacement field and the electron-electron interactions, manifest in tunnelling transport. This way, we shed light on BLG material parameters while opening the field for using the dots' rich spin and valley multiplets for quantum information.

1) Theory of tunneling spectra for a few-electron bilayer graphene quantum dot, A. Knothe, L. Glazman, V. Fal'ko, arXiv:2104.03399 2) Probing two-electron multiplets in bilayer graphene quantum dots, S. Möller, L. Banszerus, A. Knothe, L. Glazman, V. Fal'ko, C. Stampfer, et. al, arXiv:2106.08405 3) Quartet states in two-electron quantum dots in bilayer graphene, A. Knothe, V. Fal'ko, PRB 101, 235423 (2020)

CPP 1.5   Mon 12:15   H3

Unconventional Superconductivity in Magic-Angle Twisted Trilayer Graphene — ●Ammon Fischer — Institute for Theory of Statistical Physics, RWTH Aachen University

Magic-angle twisted trilayer graphene (MATTG) recently emerged as a highly tunable platform for studying correlated phases of matter, such as correlated insulators and superconductivity. Superconductivity occurs in a range of doping levels that is bounded by van Hove singularities which stimulates the debate of the origin and nature of superconductivity in this material. In this work, we discuss the role of spin-fluctuations arising from atomic-scale correlations in MATTG for the superconducting state. We show that in a phase diagram as function of doping (ν) and temperature, nematic superconducting regions are surrounded by ferromagnetic states and that a superconducting dome with $T_c \approx 2$ K appears between the integer fillings $\nu = -2$ and $\nu = -3$. Applying a perpendicular electric field enhances superconductivity on the electron-doped side which we relate to changes in the spin-fluctuation spectrum. We show that the nematic unconventional superconductivity leads to pronounced signatures in the local density of states detectable by scanning tunneling spectroscopy measurements.

CPP 1.6   Mon 12:30   H3

Twist angle dependent proximity induced spin-orbit coupling in graphene/transition-metal dichalcogenide heterostructures — ●Thomas Naimer[1], Klaus Zollner[1], Martin Gmitra[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, P. J. Šafárik University in Košice, 04001 Košice, Slovakia

We investigate proximity-induced spin-orbit coupling (SOC) in graphene on the four transition-metal dichalcogenides (TMDCs) MoS₂, WS₂, MoSe₂ and WSe₂ from first principles. By using different supercells of graphene/TMDC heterostructures we provide systematic insight on the effect of twist angles on the low energy Dirac spectrum. We find that the exact position of the Dirac cone within the TMDC band gap depends linearly on the biaxial strain applied to the graphene. From this relation we extrapolate the zero-strain band offset and correct the band offsets of all calculations by employing a transverse electric field across the heterostructure. The corrected results

reveal massive twist angle tunability of both the magnitude and flavor of proximity induced SOC: We observe a peak in SOC at approximately 19° twist angle and vanishing SOC at 30°. This work was supported by ENB "Topologische Isolatoren" and SFB 1277.

CPP 1.7   Mon 12:45   H3
Predicting the adsorption of alkali metals on 2D materials — Maofeng Dou and •Maria Fyta — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

The adsorption of alkali metal atoms on two-dimensional transition metal dichalcogenides (2D TMDCs) is investigated using quantum-mechanical calculations. Specifically, we evaluate the adsorption char-

acteristics of Li on 2D TMDCs through the respective adsorption energies. We decompose these energies into separate components in order to fundamentally understand the adsorption process. The adsorption energies of lithium on 2D TMDCs were found to strongly and linearly correlate with the energy of the lowest unoccupied states of the materials. Accordingly, we propose and demonstrate the use of this energy as a descriptor for predicting adsorption energies. We further proceed with additional 2D TMDCs and adsorbed alkali atoms in order to generate a database that allows us to learn and make predictions. Our results strongly support the use of the energy of the lowest unoccupied states as a novel efficient descriptor for a data-driven design of materials with pre-selected properties and functions for target applications.

CPP 2: Hydrogels and Microgels

Time: Monday 13:30–14:30   Location: H1

Invited Talk   CPP 2.1   Mon 13:30   H1
On the permeability of dense polymer membranes — •Joachim Dzubiella — Institute of Physics, Freiburg University

The permeability of polymers for the selective transport of molecular penetrants (drugs, toxins, reactants, etc.) is a central property in the design of soft functional materials. However, the permeation of dense and hydrated polymer membranes is a complex molecular- level phenomenon, and our understanding of the underlying physicochemical principles is still very limited. Here, I present our recent modeling efforts using coarse-grained as well as atomistic computer simulations in combination with the linear-response solution-diffusion model to understand and quantify the permeability of dense polymer (networks). Our work reveals some universal physical principles, such as strong solute partitioning-diffusion cancellation effects for a wide parameter regime, as well as significant 'chemical' effects (such as solute polarity and shape) which all contribute to the control of permeability. The gained insights enable us to formulate semi-empirical rules and scaling laws to potentially describe and extrapolate the permeability also for other polymer/solute systems.

CPP 2.2   Mon 14:00   H1
Phase behavior of ultra-soft spheres shows stable bcc lattices — •Andrea Scotti — Institute of Physical Chemistry RWTH Aachen University

The phase behavior of super-soft spheres is explored using solutions of ultra-low crosslinked poly(N-isopropylacrylamide) based microgels as a model system. For these microgels, the effects of the electric charges on their surfaces can be neglected and, therefore, only the role of softness on the phase behavior is investigated. The samples show a liquid-to-crystal transition at higher volume fraction with respect to both hard spheres and stiffer microgels. Furthermore, stable body centered cubic (bcc) crystals are observed in addition to the expected face centered

cubic (fcc) crystals. Small-angle X-ray and neutron scattering with contrast variation allow the characterization of both the microgel-to-microgel distance, and the architecture of single microgels in crowded solutions. The measurements reveal that the stable bcc crystals depend on the interplay between the collapse and the interpenetration of the external shell of the ultra-low crosslinked microgels.

CPP 2.3   Mon 14:15   H1
Co-polymerization of PNIPAM microgels with Dopamine Methacrylamide to increase adhesive properties — •Sandra Forg[1], Alexandra Karbacher[1], Regine von Klitzing[1], Zhishuang Ye[2], and Xuhong Guo[2] — [1]Soft Matter at Interfaces (SMI), Technical University of Darmstadt, Germany — [2]School of Chemical Engineering, East China University of Science and Technology, China

Microgels are cross-linked polymer particles, which are highly swollen in solvents such as water. One of those microgels is the stimuli-responsive PNIPAM, which undergoes deswelling when heated above its LCST at 32°C. The co-polymerization of PNIPAM is a well-defined technique to design unique microgel systems.

Dopamine methacrylamide (DMA) is a catechol-based monomer, which is main responsible for the adhesive properties of marine organisms. Combining the stimuli-responsiveness of PNIPAM with the adhesive properties of DMA bears a huge potential for biomedicine.

In literature the formation mechanisms of such microgel networks are shown. Furthermore, it is well-known that such catechol-based monomers like DMA have a high radical scavenging ability and thus cross-link the microgel. But, so far, a detailed understanding of the co-polymerization is missing. Therefore, the reaction kinetics of DMA during the microgel synthesis are presented in this work. The built-in DMA was verified by UV-VIS standard addition and NMR spectroscopy. First adhesion tests under water will be presented.

CPP 3: Polymer Physics

Time: Monday 13:30–16:15   Location: H3

Invited Talk   CPP 3.1   Mon 13:30   H3
Emulsion Templating: Unexpected Morphology of Monodisperse Macroporous Polystyrene — •Cosima Stubenrauch[1], Lukas Koch[1], Sophia Botsch[1], and Wiebke Drenckhan[2] — [1]Institut für Physikalische Chemie, Universität Stuttgart, Deutschland — [2]Institute Charles Sadron, CNRS Strasbourg, Frankreich

We start with a monodisperse, hexagonally close-packed water-in-monomer high internal phase emulsion (HIPE). The polymerization of the continuous monomer phase with a water-soluble initiator leads to a monodisperse, macroporous polymer with an unexpected morphology: the pore cross-sections of this material are closed hexagons and the pore walls consist of three distinctive layers. Though this morphology has already been observed for two different systems, the mechanism leading to it has not been identified yet. Based on new experimental results we propose a surfactant-driven mechanism: excess surfactant is dissolved in the continuous phase, where it emulsifies water from the emulsion droplets. When the polymerization is initiated from the interface, the continuous phase becomes a poor solvent for both the

surfactant and the emulsified water. As a consequence, they "flee" from the site of the polymerization (1) towards the water/monomer interface or (2) into the yet unpolymerized inside of the continuous phase. The first process may cause the emulsion droplets to change their shape from spherical to polyhedral and the second process may be responsible for the formation of the three observed layers in the pore wall. We will (a) discuss both processes in detail and (b) present the experimental results that clearly support them.

CPP 3.2   Mon 14:00   H3
Dissociation degree and pKa value of polyacid systems in solution and coatings determined by FTIR titration — Luise Wirth[1,2], Birgit Urban[1], Carolin Naas[1,2], and •Martin Müller[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Department Functional Colloidal Materials, Hohe Str. 6, D-01069 Dresden, Germany — [2]Technische Universität Dresden, Department Chemistry and Food Chemistry, D-01062 Dresden, Germany

Dissociation degree a and pKa of poly(acrylic acid) (PAA) and pro-

pionic acid (PA) 0.1 M solutions were determined by FTIR titration and potentiometric (POT) titration concept. Increasing subsequently the pH value from 2 to 12 by adding 1 M NaOH portions, FTIR spectra of PA and PAA show decrease of n(C=O) and increase of n(COO-) band due to carboxyl (COOH) and carboxylate (COO-) groups, respectively. From the respective normalized band integrals A, the dissociation degree aIR=ACOO-/(ACOOH+ACOO-) can be calculated. pH was plotted versus aIR and fitted by pH=pKa+B log(aIR/(1-aIR)) related to Henderson-Hasselbalch equation with fit parameters pKa and empirical cooperativity factor B. The slight pKa deviation found for FTIR and POT titration, the respective deviation between monomeric PA and polymeric PAA and the PAA molecular weight trend (PAA-2K, PAA-50K, PAA-450K) are discussed based on the known two-phase model of polyelectrolyte solutions including Gibbs-Donnan potential concept. Furthermore, aIR of PAA within consecutively adsorbed polycation/PAA multilayer coatings was determined by FTIR titration showing significant effect of the outermost polyelectrolyte layer.

CPP 3.3   Mon 14:15   H3

New nanoscale gradient copolymer films fabricated via initiated chemical vapor deposition (iCVD) — ●Stefan Schröder, Alexander M. Hinz, Oleksandr Polonskyi, Thomas Strunskus, and Franz Faupel — Kiel University, Institute for Materials Science, 24143 Kiel, Germany

Many structures found in the natural world are based on organic gradients. To reproduce these structures, polymers are an excellent choice, as they also enable the formation of gradient copolymers. This study reports on the fabrication of such gradient copolymers in the form of thin films via initiated chemical vapor deposition (iCVD). Solvent-free deposition and the mild deposition conditions are only two of the advantages of iCVD in order to produce high-quality polymer thin films on large-area substrates, complex geometries as well as temperature-sensitive samples. In addition, the process enables the combination of comonomers which typically lack a common solvent. For the transfer of the gradient film approach to the lower nanoscale, a detailed understanding and control of the vapor phase kinetics are required. This is solved in this study by a novel in-situ quadrupole mass spectrometry (QMS) extension combined with supporting ab-initio/density functional theory (DFT) calculations. It offers a better insight into the underlying reaction kinetics and enables enhances process control during the deposition. This facilitates the fabrication of gradient copolymer films with film thicknesses below 30 nm. They show completly new physical and chemical properties, which cannot be obtained with materials currently in use.

Invited Talk   CPP 3.4   Mon 14:30   H3
Structural Transitions of Molecules on Surfaces — ●Angelika Kühnle — Physical Chemistry I, Department of Chemistry, University Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Molecular self-assembly constitutes a versatile strategy to create functional molecular structures at surfaces. Conventionally, self-assembly is associated with structures in thermodynamic equilibrium. In this talk, several examples will be given for molecular structures that are explained by thermodynamic equilibrium. However, observed structures might be kinetically trapped, and structural transitions can be induced by annealing. On the (111) surface of copper, dimolybdenum tetraacetate (MoMo) molecules are shown to undergo a reversible phase transition of molecular islands (2D solid phase) into mobile molecules (2D gas phase). Interestingly, while this phase transition is usually associate with heating, the mobilization of the MoMo molecules presented here is observed upon cooling. In this talk, the molecular-scale origin of this inverse phase transition is discussed.

15 min. break

CPP 3.5   Mon 15:15   H3

Tack Properties of Pressure-Sensitive Adhesive-Coated Fiber Assemblies — ●Volker Körstgens, Jorge Corella Puertas, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

For the mechanical characterization of the adhesive bond of pressure-sensitive adhesives one has to take into account the geometry of the adherents and the kind of stress applied. We present a technique, which allows for the measurement of tack for assemblies of fibers coated with pressure-sensitive adhesives using customized cylindrical compos-

ite stamps [1]. Key element of the method is the proposed technique to achieve monolayers of parallel-aligned fibers as a fiber assembly. With the adapted probe tack test we investigated the tack properties of a polymer blend of poly(vinylpyrrolidone-co-vinylacetate) and polyethylene glycol (PEG) coated on human hair. This composition serves as a simple model system for hair styling products. The influence of different PEG contents and of the humidity on the tack is demonstrated. Nylon fibers with different diameters are studied as references. [1] V. Körstgens et al., ACS Appl. Polym. Mater. 2, 3189-3195 (2020).

CPP 3.6   Mon 15:30   H3

Thermoporometry Characterization of Mesoporous Materials: A Kernel-Based Approach — ●Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

Detailed characterization of the structure of mesoporous solids presents key insights into the tailored design for various industrial applications such as catalysis, molecular separations and adsorption, among others.

Thermoporometry, as a characterization technique, suffers from some inaccuracies which make it lag behind gas sorption for textural characterization.

Herein, we present a kernel-based approach for the thermoporometry characterization approach which accounts for a varying non-frozen layer thickness due to pore curvature and temperature and thermal fluctuations in especially, very small pores. Additionally, with the help of the serially-connected pore model (SCPM), we reveal disorder in cylindrical pores whose complex morphology results in cooperativity effects in thermodynamic phase behavior.

References [1] Enninful et 2019, Frontiers in Chemistry, doi: 10.3389/fchem.2019.00230. [2] Enninful et 2020, Microporous and Mesoporous Materials 309, 110534.

CPP 3.7   Mon 15:45   H3

Columnar Stacks of Azobenzene Stars Under Irradiation - Photoisomerization Kinetics and Light-Induced Defects — ●Markus Koch, Marina Saphiannikova, and Olga Guskova — Institute Theory of Polymers, IPF Dresden, Germany

Azobenzenes (azo) are a class of molecules that photoisomerize between their trans and cis state, causing dramatic conformational changes. These chromophores are widely used to add light-responsive properties to various microscopic or macroscopic systems. The object of this study is a star-shaped molecule (TrisAzo) containing three azo groups connected via a BTA group. TrisAzo not only has a rich photoisomerization behavior [1]. In polar media, these molecules self-assemble into supramolecular structures, that undergo a reversible morphological transition upon UV-Vis light irradiation [2]. Our study focuses on modeling these systems via fully atomistic MD simulations. In particular, we investigate the effects of UV-Vis light on columnar TrisAzo stacks [3]. Using a detailed simulation approach, we can closely reproduce the photoisomerization kinetics in these systems. Moreover, the results demonstrate how light induces defects in the columns and how this is related to the intermolecular interactions of stacked TrisAzo molecules. We thank the German Research Foundation (DFG) for financial support, project GU 1510/5-1.
[1] M. Koch et al. J. Phys. Chem. B 121 (37), 8854-8867 (2017)
[2] S. Lee et al. Langmuir 29 (19), 5869-5877 (2013)
[3] M. Koch et al. Langmuir 35 (45), 14659-14669 (2019)

CPP 3.8   Mon 16:00   H3

Free energy considerations in confined heterocatalysis in a supported ionic liquid phase — ●Takeshi Kobayashi[1], Hamzeh Kraus[2], Felix Ziegler[3], Michael Buchmeiser[3], Niels Hansen[2], and Maria Fyta[1] — [1]Institute for Computational Physics, University of Stuttgart — [2]Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart — [3]Institute of Polymer Chemistry, University of Stuttgart

The high potential of performing heterocatalysis in a confined mesoporous media within a supported ionic liquid phase (SILP) is studied using Molecular Dynamics (MD) simulations. Specifically, we investigate the possibility of immobilizing catalytic molecules in confined media in a biphasic solution consisting of an ionic liquid (IL) and heptane as the second phase within a pore with a lateral size of about 5 nm. Divalent cationic Ru-alkylidene N-heterocyclic carbene catalysts are placed in the solution. We were able to monitor the immobilization of the catalysts within the IL for achieving higher turnover rates in the catalytic reactions. We further analyze the accumulation and diffusion of the molecules within the pore, the influence of steric and IL-specific

effects, the structuring of a solvent environment, and their synergistic interactions with the catalytic molecules. The free energy calculations reveal that the catalytic reaction must occur at the interface between the heptane and the IL. Our investigations are supported by experi-

mental evidence and provide a deeper understanding of the inherent details that control a rational design of a linker-free catalyst immobilization in nanometer-sized templates for catalytic applications.

CPP 4: Focus: The Physics of Adaptive Polymer Networks

organized by Regine von Klitzing (TU Darmstadt) und Christian Holm (Universität Stuttgart).

Adaptive polymer networks and gels represent soft materials with dimensional stability and viscoelasticity, which can assume different states due to changes in environmental conditions. This makes them promising candidate materials for a variety of applications, such as membranes for separation techniques or perm-selective membranes, and sensors and actuators. A particularly versatile class of adaptive gels are amphiphilic networks, which combine components that swell selectively in different media. The investigation of these amphiphilic co-networks represents a topic of high current relevance in polymer sciences, which has been coordinated in Germany by the research group FOR2811 since 2019 (www.for2811.uni-mainz.de).

Time: Tuesday 10:00–12:45 Location: H3

Invited Talk CPP 4.1 Tue 10:00 H3

Adaptable amphiphilic co-networks: structure and properties in relation with multi-quantum NMR — •Michael Lang[1], Reinhard Scholz[1], Lucas Löser[2], Carolin Bunk[1], Frank Böhme[1], and Kay Saalwächter[2] — [1]Leibniz-Institut für Polymerforschung, Hohe Straße 6, 01069 Dresden, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physics - NMR Group, Betty-Heimann-Str. 7, 06120 Halle, Germany

Amphiphilic co-networks made by the hetero-complementary coupling of four arm star polymers are an interesting model system to understand the physics of adaptive co-networks and currently the focus of the DFG research unit FOR2811 in which we participate. We analyze these model networks in different states (preparation in co-solvent, swollen state, and "switched" states where one type of polymer is swollen and the other collapsed) with large scale Monte-Carlo simulations and experiments. We discuss the degree of swelling, the scattering function, chain extensions, etc. of these model systems briefly. A particular focus is put on data and models regarding proton multiple-quantum NMR. After a brief tutorial on what can be analyzed with this method, we sketch analytical models for NMR order parameters in a particular state and compare with the availabe simulation or experimental data in these states. This analysis provides useful information on the time average local properties of individual network strands including the strain distribution of network strands. Such information is hardly accessible with alternative methods and allows even for the analysis of cyclic network defects under appropriate conditions.

Invited Talk CPP 4.2 Tue 10:30 H3

Adaptive networks through supramolecular interactions — •Ilja Voets — Department of Chemical Engineering and Chemistry & Institute for Complex Molecular Systems, Eindhoven University of Technology

Supramolecular interactions offer a powerful tool to modulate self-assembly pathways to generate dynamic materials with adaptive properties. In this lecture I will showcase two versatile, supramolecular approaches to generate adaptive, polymer-based materials, based on electrostatically driven co-assembly of ionic-neutral block copolymers and on amphiphilic copolymers equipped with suitable motifs, such as C3-symmetrical discotics based on benzene-1,3,5-tricarboxamides (BTAs), encoded to form one-dimensional helical 'stacks'. I will discuss the structure and properties of the micellar and fibrillar objects that these materials form in dilute aqueous solution, and of the transient networks which emerge at elevated concentrations. Recent efforts and insights in e.g. polyelectrolyte complexation out-of-equilibrium, strain stiffening, high resolution optical imaging and templated polymerization will be addressed. In future, these concepts may be exploited to further custom-tailor gels towards a desired structure and associated mechanical response.

15 min. break

CPP 4.3 Tue 11:15 H3

Chain connectivity of tetra-PEG - tetra-PCL amphiphilic

end-linked polymer model networks — •Lucas Löser[1], Carolin Bunk[2], Frank Böhme[2], and Kay Saalwächter[1] — [1]Inst. f. Physik - NMR, Martin-Luther-Universität Halle-Wittenberg — [2]Leibnitz-Institut f. Polymerforschung Dresden e.V., Hohe Str. 6, Dresden

A new approach for the synthesis of model-like amphiphilic co-networks is introduced, and their structure analysed by static 1H time-domain nuclear magnetic resonance (NMR) methods. A novel approach of hetero-complementary end-linking [1] of two well-defined tetra-armed polyethylene glycol (PEG) stars based on Sakai et al. [2] is used and modified in a way, that amphiphilic gels are obtained. We link PEG stars with a hydrophobic poly-ϵ-caprolactone star (tetra-PCL) terminated with an oxazinone group, resulting in the formation of an amphiphilic network. By using static 1H-1H multiquantum-NMR, as initially performed by Lange et al. [3], we show that our method is capable of distinguishing different chain species in the swollen PEG-PCL networks, allowing quantification of network connectivity defects arising from the end-linking reaction of A4- and B4-type stars, as well as accurate quantification of inelastic material. The parameter space of the synthesis is explored and changes in microscopic network structure are studied depending on polymer concentration and different temperature programs during synthesis. [1] Jakisch et al. ; Macromol. Chem. Phys 2017, 219 [2] Sakai, T. et al.; Macromolecules 2008, 41 [3] Lange, F. et al.; Macromolecules 2011, 44

CPP 4.4 Tue 11:30 H3

Microscopic and macroscopic mechanical properties of amphiphilic model co-networks — •Nora Fribiczer[1], Kevin Hagmann[2], Carolin Bunk[3], Sebastian Seiffert[1], Regine von Klitzing[2], and Frank Böhme[3] — [1]Department of Chemistry, Johannes Gutenberg University Mainz, D-55128 Mainz — [2]Institute for condensed matter physics, Technische Universität Darmstadt, D-64289 Darmstadt — [3]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden

Amphiphilic polymer gels are composed of both hydrophilic and hydrophobic polymers, which makes their mechanical properties dependent on environmental conditions such as the solvent polarity. In this work, we present both a microscopic and macroscopic perspective of these properties using indentation atomic force microscopy and oscillatory shear rheology. With this, we aim to get a rational understanding of the interplay between the environmental conditions and the resulting mechanical properties in the bulk material and at the interface.

Next to the investigation of the mechanical properties under good and bad solvent conditions, we put special emphasis on the characterization of the gelation process during network formation. By variation of concentration and temperature the reactivity and network topology can be controlled due to the use of an innovative bi-functional coupling agent which connects the hydrophilic tetra-PEG and the hydrophobic tetra-PCL. Monitoring the network formation using shear rheology allows for determination of the respective gel points, which coincide with results obtained from nuclear magnetic resonance spectroscopy.

Invited Talk CPP 4.5 Tue 11:45 H3

Tunable self-assembled hydrogels from block copolymers with thermoresponsive and pH-responsive blocks — •Christine M. Papadakis[1], Florian A. Jung[1], and Constantinos Tsitsilianis[2] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Chemical Engineering, University of Patras, Greece

Pentablock terpolymers with thermoresponsive end blocks and a pH-responsive middle block form hydrogels in aqueous environment. By altering the stability of the crosslinks and the degree of bridging, the responsivities afford numerous possibilities to tune the mechanical properties. Small-angle neutron scattering revealed the underlying mesoscopic structures in dependence on temperature and the pH value [1]. The thin film geometry allows studying the microphase-separated structures in the dry state and during swelling in the vapor of water or organic solvents in situ using grazing-incidence small-angle X-ray scattering. The results reveal the role of the dielectric properties of the solvent for microphase separation and hydrogel formation [2].

[1] C. Tsitsilianis et al., *Macromolecules* **2018**, *51*, 2169. F. A. Jung et al., *Macromolecules* **2019**, *52*, 9746. M. M. S. Lencina, et al., *ACS Appl. Polym. Mater.* **2021**, *3*, 819.
[2] F. A. Jung et al., *Macromolecules* **2020**, *53*, 6255.

CPP 4.6   Tue 12:15   H3

Structural characterization of covalently connected amphiphilic star polymer conetworks — •Reinhard Scholz[1], Lucas Löser[2], Kay Saalwächter[2], Carolin Bunk[1], Frank Böhme[1], and Michael Lang[1] — [1]Leibniz Institut für Polymerforschung, 01005 Dresden, Germany — [2]Institut für Physik - NMR, Martin-Luther-Uniweristät Halle-Wittenberg, 061120 Halle, Germany

Polymer networks consisting of complementary four functional stars of poly ethylene glycol (PEG) and poly caprolactone (PCL) were synthesized via covalent coupling of complementary end groups. The equilibrium swelling in various solvents revealed either compatibility of both polymer components with good solvents for both components like in toluene, or a reduced swelling in solvents like THF or water, representing selective solvents for the PEG component only. Complementary X-ray scattering studies allowed to assign the structure factor to a swollen conetwork (in toluene), or to a swollen PEG component connecting embedded clusters of PCL (in THF or water). These experimental results were accompanied by simulations of network formation as a function of polymer concentration during preparation, and subsequent swelling in a cosolvent or a selective solvent. The calculated structure factor arising from the simulated model networks reveals a typical length scale for the size and distance of the PCL clusters, in reasonable agreement with the dependence of the observed scattering intensity on wave vector.

CPP 4.7   Tue 12:30   H3

From four-arm block copolymers to electrostatically cross-linked gels — •Peter Johannes Mons[1], Nora Fribiczer[2], David Beyer[3], Felix Helmut Schacher[1], Sebastian Seiffert[2], and Christian Holm[3] — [1]Institute of Organic Chemistry and Macromolecular Chemistry, Friedrich-Schiller-University Jena, D-07743 Jena — [2]Department of Chemistry, Johannes Gutenberg-University Mainz, D-55128 Mainz — [3]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart

Reversibly electrostatically cross-linked polymer networks composed of oppositely charged four-armed star block copolymers feature favorable properties such as environmentally sensitive viscoelasticity and selective permeability. In this work, we present different double hydrophilic star-shaped block copolymers with oppositely charged polyelectrolytes that can form electrostatically cross-linked gels. A new class of reversible double hydrophilic or amphiphilic networks can be synthesized based on these gels.

The four-armed copolymers consist of a PEG-core block extended with sulfonated polystyrene or N,N-dimethylaminopropyl acrylamide (DMAPAa). The sulfonated polystyrene block carries a permanent anionic charge whereas the DMAPAa block carries a permanent cationic or pH-tunable charge. The gel formation upon mixing these block copolymers was verified by shear rheology, which showed a high dependence of the gel strength on the presence of counterions. Coarse-grained molecular dynamics simulations support the picture of well-gelated networks and give insight into the molecular conformations.

CPP 5: Poster Session I

Electrical, Dieelectrical and Optical Properties of Thin Films (1-7); Hybrid and Perovskite Photovoltaics (8-13); Organic Electronics and Photovoltaics (14-16); Molecular Electronics and Excited State Properties (17-19).

Time: Tuesday 17:30–19:30   Location: P

CPP 5.1   Tue 17:30   P

Thermal degradation of EMIM DCA post-treated PEDOT:PSS thermoelectric thin films, investigated via in-situ GISAXS — •Anna Lena Oechsle[1], Julian E. Heger[1], Nian Li[1], Shanshan Yin[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]ELETTRA Sincrotrone Trieste S. C. p. A., 34149 Basovizza TS, Italy — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

The constantly increasing energy demand raises the need for renewable energies and the reduction of energy dissipation. Thermoelectric materials are promising in terms of waste heat recovery and the use of solar thermal energy, as they enable the direct conversion of a temperature gradient into electrical power. Nowadays great research focus is especially on thermoelectric polymers, as they are low or nontoxic, lightweight, flexible and allow a low-cost, large-scale solution-based production of thin films. In this work we show the positive influence of EMIM DCA post-treatment on the Seebeck coefficient and electrical conductivity of PEDOT:PSS thin films. However, for possible future applications it is also important to understand the behavior of these films during long-term operation at elevated temperature. Therefore, we reveal occurring morphology changes with in-situ GISAXS measurements of these films and try to link them to the observed decrease in the electrical conductivity.

CPP 5.2   Tue 17:30   P

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-Franck-Str. 1, 85748 Garching, Germany

Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially* 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. It is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the interdependence of parameters as a function of charge carrier concentration. In this work, we adopt a combination of DMSO addition and subsequent DMSO/salt mixture post-treatment to improve the TE performance of PEDOT: PSS thin films. Results show that the as-obtained PEDOT: PSS film presents a maximum PF of 105.2 *W(m-1K-2), which is ~1750-fold leap larger than that of pristine film. The origin and mechanism of the underlying improvement are systematically investigated by various characterizations to gain a more profound understanding of the fundamental nature of the modified PEDOT: PSS films.

CPP 5.3   Tue 17:30   P

Measurement setup to characterize thermoelectric polymer thin films — •Simon Wegener[1], Anna Lena Oechsle[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching,

Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

The growing need to save fossil resources requires, besides their substitution, also their effective usage. This usage is mostly limited by the high amounts of wasted heat in the conversion from chemical energy to mechanical or electrical energy. Thermoelectric (TE) materials are a promising way to make use of this wasted energy. Particularly, they can be used in a wide range of applications to generate electricity. Nevertheless, these materials show lots of room for improvement in terms of their output power. Therefore, with our work, we aim to construct a setup, which focuses especially on the measurement of polymer-based TE materials for low-temperature applications. This setup consists of two mounting plates that can be heated or cooled individually to determine the Seebeck coefficient. Additionally, a van der Pauw measurement can be done to find the electrical conductivity of the sample. By this, the setup will enable the user to rapidly characterize samples by its TE power factor.

CPP 5.4   Tue 17:30   P

Tailoring the Optical Properties of Sputter-Deposited Gold Nanostructures on Nanostructured Titanium Dioxide Templates — •Suzhe Liang[1], Wei Chen[1], Shanshan Yin[1], Simon J. Schaper[1], Jonas Drewes[2], Niko Carstens[2], Thomas Strunskus[2], Franz Faupel[2], Marc Gensch[1,3], Matthias Schwartzkopf[3], Stenphan V. Roth[3,4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Garching, Germany — [2]CAU,Kiel, Germany — [3]DESY, Hamburg, Germany — [4]KTH, Stockholm, Sweden — [5]MLZ, TU München, Garching, Germany

Au/TiO2 nanohybrid materials have attracted significant attention due to the outstanding optical, photocatalytic and photovoltaic performance. We use customized polymer templating to achieve TiO2 nanostructures with different morphologies. Au/TiO2 hybrid thin films are fabricated by sputter deposition. An in-depth understanding of the Au morphology on the TiO2 templates is achieved with in situ GISAXS during the sputter deposition. The resulting Au nanostructure is largely influenced by the TiO2 template morphology. Based on the detailed understanding of the Au growth process, characteristic distances can be selected to achieve tailored Au nanostructures at different Au loadings. For selected sputter-deposited Au/TiO2 hybrid thin films, the optical response with a tailored localized surface plasmon resonance is demonstrated.

CPP 5.5   Tue 17:30   P

Sputter-depostion vs. spraying: effect of doping technique on the structural and thermoelectric properties of P3HT-based thin films — •Benedikt Sochor[1], Constantin Harder[1], Anna-Lena Oechsle[2], Matthias Schwartzkopf[1], Alexei Vorobiev[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Technical University Munich, Physics Department, James-Franck-Str. 1, 85748 Garching, Germany — [3]Institue Laue-Langevin, 71 Avenue des Martyrs, 38042 Grenoble Cedex 9, France — [4]KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden

Poly(3-hexylthiophen-2,5-diyl) (P3HT) is one of the most prominent semiconducting, conjugated polymers in the fields of organic electronics and photovoltaics. This study aims for correlating process and fabrication parameters and the structural changes with the overall thermoelectric performance of P3HT and P3HT:PMMA films. Especially, we focus on two routes of gold (Au) doping, namely sputter and spray deposition techniques. The structure of the resulting polymer composites indicated distinct differences whether the gold is sprayed or grown on the surface as shown by AFM as well as neutrons and X-ray reflectivity measurements. During in situ GISAXS experiments, the growth and structure of the gold particles was mapped, which indicated the presence of sub-nanometer sized gold clusters in case of sputter deposition.

CPP 5.6   Tue 17:30   P

Hybrid energy harvester based on triboelectric nanogenerator and solar cell — •Tianxiao Xiao[1], Wei Chen[1], Wei Cao[1], and Peter Müller-Buschbaum[1,2] — [1]Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße. 1, 85748 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 tribo-electrification 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 based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 5.7   Tue 17:30   P

Colloidal photonic crystal slabs toward enhanced photoconductivity — •Swagato Sarkar[1], Vaibhav Gupta[2], and Tobias A. F. König[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden e.V. (IPF), Institute for Physical Chemistry and Polymer Physics, Hohe Str. 6, 01069 Dresden, Germany — [2]Institute of Particle Technology, Friedrich-Alexander University Erlangen-Nürnberg, Cauerstrasse 4, 91058 Erlangen, Germany — [3]Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden 01062 Dresden, Germany

In the present work, a fusion of interference lithography (IL) and nanosphere imprint lithography [Gupta, König, Fery, ACS Appl. Mater. Interfaces 2019, 11, 28189.] on various target substrates ranging from carbon film on transmission electron microscope grid to inorganic and dopable polymer semiconductor is reported. 1D colloidal photonic crystals are printed with 75% yield on the centimeter scale using colloidal ink and an IL-produced polydimethylsiloxane stamp. Atomically smooth facet, single-crystalline, and monodisperse colloidal building blocks of gold (Au) nanoparticles can produce 1D plasmonic grating on top of a titanium dioxide (TiO2) slab waveguide, producing waveguide-plasmon polariton [Sarkar, Fery, König, Adv. Funct. Mater. 2021, 31, 2011099.] modes with superior 10 nm spectral linewidth. Plasmon-induced hot electrons are confirmed via two-terminal current measurements resulting in increased photoresponsivity as well as enhanced photocatalytic degradation of methyl orange (MO) dye molecules.

CPP 5.8   Tue 17:30   P

Upscaling Perovskite: Optoelectronics and Morphology of Slot-Die Coated Solar cells — •Andrea Vitaloni[1], Lennart K. Reb[1], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) have attracted increasing attention in research and industry due to their high efficiency, low material cost, and simple solution-based fabrication process. Additionally, the possibility to fabricate flexible and thin solar cells creates new opportunities compared to traditional solar modules.

In laboratory devices, the efficiency already exceeds 25% and is comparable with c-Si. However, one of the most important steps towards commercialization is the upscaling of the PSCs production to larger areas. Slot-die coating is considered to be one of the most promising technology, being a fast process with minimum material consumption and waste. Furthermore, the highly tuneable perovskite ink composition strongly determines kinetic processes during film formation and the final morphology.

We vary the composition of MAPI inks and analyze the printed perovskite thin-films and derived solar cells with spectroscopic and X-ray scattering methods. The focus is on developing a comprehensive understanding of the slot-die coating process for printed, flexible, and high-efficiency PSCs.

CPP 5.9   Tue 17:30   P

In-Operando study of humidity on the performance of perovskite solar cell — •Kun Sun[1] and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-

Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSCs) are one of the most promising photovoltaic technologies and reached a certified 25.2% efficiency owing to their tuneable bandgap, high carrier mobility, long diffusion length and so on. The long-term operational stability of PSCs, however, has been not investigated. Herein, we probe the structure change with grazing-incidence small-angle scattering (GISAXS) under high humidity. Also, the solar cell parameters are obtained simultaneously during the device operation. We find that PSCs fabricated with and without caesium iodide (CsI) show differences in the device degradation and morphology change in the perovskite layer. The decrease of open-circuit voltage (VOC) can be attributed to the morphology changes and the evolution of crystallize grain size. With the additive of CsI, solar cells show slow decay of VOC, which is correlated to improved morphology of active layer and passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology change combined with solar cell parameters during the device operation.

CPP 5.10   Tue 17:30   P

Tailoring the orientation of perovskite crystals via adding two-dimensional polymorphs for perovskite solar cells — •Renjun Guo[1], Ali Buyruk[2], Xinyu Jiang[1], Wei Chen[1], Lennart K. Reb[1], Manuel A. Scheel[1], Tayebeh Ameri[2], and Peter Müller-Buschbaum[1] — [1]Physik-Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Chemie-Department, Ludwig-Maximilians-Universität München, Butenandtstr. 5-13 (E), 81377 München, Germany

Due to their outstanding properties, organic-inorganic perovskite materials are gaining increasing attention for their use in high-performance solar cells. Finding an effective method of defect passivation is thought to be a promising path for advancements toward narrowing the distribution of the power conversion efficiency (PCE) values, as measured by the spread in the PCE over different devices fabricated under identical conditions, for easier commercialization. We add 2*(4*fluoroph-enyl)ethyl ammonium iodide (p-f-PEAI) into the bulk of a mixed cation lead halide perovskite film in this study. The addition of the appropriate amount of p-f-PEAI affects the preference orientation of the perovskite crystals, increases the strength of the crystal texturing, and reduces non-radiative charge recombination. As a result, we achieve a tighter range of the PCE of perovskite solar cells (PSCs) without losing the PCE values obtained [1].

[1] Guo et al. J. Phys. Energy 2, 034005 (2020)

CPP 5.11   Tue 17:30   P

Fabrication and characterisation of slot-die coated formamidinium-cesium lead iodide perovskite solar cells — •Alexander Franz Weinzierl[1], Manuel A. Scheel[1], Lennart K. Reb[1], and Peter Müller-Buschbaum[1,2] — [1]Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite solar cells (PSC) are a promising candidate to evolve the solar energy market due to high energy conversion efficiencies and low cost material usage. However, many perovskite absorber compositions suffer from long-term stability problems. Perovskites, composited of formamidinium/caesium lead iodide/bromide (FACs), as the active layer of such solar cells are promising to overcome this issue. Crucial for FACs is the development of a solvent system together with an optimised printing process enabling to produce highly homogeneous layers and, as a result, cells with high performance and low degradation. To achieve this outcome, slot-die coating is examined for depositing the Perovskite ink, especially, since this printing technique is transferable to the scale-up of PSCs towards commercial sizes. In this work inverted slot-die coated FACs solar cells are produced with different solvents. Their film morphology is investigated by microscopy, X-ray diffraction and GIWAXS. Moreover, the cells are characterised and compared via their respective current-voltage characteristic, giving insight into the performance parameters.

CPP 5.12   Tue 17:30   P

The Influence of CsBr on Crystal Orientation and Optoelectronic Properties of MAPbI3-based Solar Cells — •Yuqin Zou and Peter Müller-Buschbaum — Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, James-

Franck-Straße 1, 85748 Garching, Germany.

Crystal orientations are closely related to the behavior of the photo-generated charge carrier and vital for controlling the optoelectronic properties of perovskite solar cells. Herein, we propose a facile approach to reveal the effect of lattice plane orientations on the charge carrier kinetics via constructing CsBr doped mixed-cation perovskite phases. Through GIWAXS measurements, we systematically investigate the crystallographic properties of mixed perovskite films in the microscopic scales and reveal the effect of the extrinsic CsBr doping on the stacking behavior of the lattice planes. And 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 5.13   Tue 17:30   P

Self-assembled Hybrid Plasmonic Nanostructures for Perovskite Solar Cells — •Tianfu Guan, Renjun Guo, Lennart K. Reb, Suzhe Liang, 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 gained great interest in various fields, owning 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. GISAXS is used to study the quality of the plasmonic structure interface in terms of contact area with the perovskite film. GIWAXS is used to probe the crystalline structure of the perovskite active layers.

CPP 5.14   Tue 17:30   P

Effect of chemical modification on crystal structure and thermal properties of Polydiketopyrrolopyrrole Copolymers — •Robert Kahl[1], Gert Krauss[2], Andreas Erhardt[2], Oleksandr Dolynchuk[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany — [2]Applied Functional Polymers, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth, Germany

Polydiketopyrrolopyrrole (PDPP) copolymers are second-generation semiconducting polymers that gained interest due to their superior performance in transistors and solar cells. Their chemical structure consisting of a DPP core with flanking units and/or co-monomers offers many opportunities to tune the optoelectronic properties by introducing chemical modifications. Here we investigated the thermal properties and crystal structure in bulk (DSC, TGA, WAXS) and in thin films (GIWAXS, AFM) of three PDPPs: PDPP[T]$_2${2-HD}$_2$-T{DEG} (PDPP1) with thiophene flanking units and an additional OEG side chain, PDPP[Py]$_2${2-HD}$_2$-T (PDPP2) with pyridine flanking units and PDPP[T]$_2${2-HD}$_2$-T (PDPP3) with thiophene flanking units. PDPP3 shows only sanidic liquid crystalline order. PDPP1 shows crystalline order and a significantly lower melting temperature than PDPP2 and PDPP3. PDPP2 shows the most WAXS peaks, but has poor thermal stability. Our results demonstrate that thermal properties and ordering ability can be significantly influenced by introducing seemingly minor changes to the chemical structure of PDPPs.

CPP 5.15   Tue 17:30   P

Following the morphology formation of printed non-fullerene active layers for solar cells — •Xinyu Jiang[1], Suo Tu[1], Manuel A. Scheel[1], Shanshan Yin[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, Garching, Germany — [2]DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements in the past few years, however, traditional laboratory deposition methods like spin coating are limited to small-scale production. Encouragingly, the emergence of printing techniques and the development of in-situ observation technology open new windows for lager-area device manufacturing and inspection of the formation process of the printed active layer, respectively. We fabricate an active layer, which contains a donor polymer (PDTBT2T-FTBDT) and a non-fullerene acceptor (BTP-4F) with slot-die coating. The structure formation of the polymer domains is followed in-situ during the printing process with GIWAXS and UV-Vis spectroscopy measurements, respectively. Thus, structure evolution is coupled with optical properties during the printing process, thereby providing an understanding of the film formation kinetics of non-fullerene organic BHJ thin films.

CPP 5.16   Tue 17:30   P

Influence of non-halogenated solvents on the morphology and stability of PTQ10:BTP-4F organic solar cells —
•Lukas Spanier[1], Renjun Guo[1], Julian Heger[1], Yuqin Zou[1], Matthias Nuber[2], Matthias Schwartzkopf[3], David Toth[4], Rachid Houssaini[4], Hristo Iglev[2], Reinhard Kienberger[2], Achim Hartschuh[4], Stephan Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]TU München, Lehrstuhl für Laser- und Röntgenphysik, Garching, Germany — [3]Deutsches Elektronen-Synchrotron (DESY), FS-PE, Hamburg, Germany — [4]Ludwig-Maximilians-Universität München, Department Chemie und CeNS, Munich, Germany

Organic solar cells (OSCs) 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 reduced performance. This can be partially reversed by raising the temperature of the solvents during formation of the bulk-heterojunction (BHJ).
We investigate and compare the changes in morphology and performance stability of PTQ10:BTP-4F OSCs processed from various solvents, utilising operando grazing-incidence X-ray scattering during illumination and solar cell operation. We further show the impact of solvent composition on the charge carrier dynamics in the respective BHJs using time-resolved transient absorption spectroscopy.

CPP 5.17   Tue 17:30   P

Polarization Resolved Optical Spectroscopy of PEN:PFP Charge-Transfer Excitons —
•Darius Günder[1], Ana M. Valencia[2,3], Michele Guerrini[2,3], Tobias Breuer[1], Caterina Cocchi[2,3], and Gregor Witte[1] — [1]Molekulare Festkörperphysik, Philipps-Universität Marburg — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [3]Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof

Charge-transfer excitons (CTX) occurring at molecular donor/acceptor interfaces are considered important intermediates for charge separation in photovoltaic devices. Co-crystalline pentacene:perfluoro-pentacene (PEN:PFP) films can be prepared with different molecular orientation on SiO2 and graphene substrates [1] and thus are well-suited model systems for detailed structure-property investigations of such CTX states. In this study, such crystalline PEN:PFP films with different molecular orientations are used to perform polarization and angular resolved UV/Vis absorption spectroscopy, in order to determine the direction of the transition dipole moment (TDM) of the CTX state, which is found to be perpendicular

to the aromatic ring planes i.e. along the stacking direction. Interestingly, this orientation is different than for the singlet excitons of unitary acene films, which can be well-described by the Kasha-model using the TDMs of the single molecule HOMO-LUMO excitations that are oriented along the M-axis and thus constitutes an important benchmark system for a refined theoretical analysis of such molecular donor/acceptor systems. [1] D'Avino et al. Chem. Mater. 32, 3, 1261-1271 (2020)

CPP 5.18   Tue 17:30   P

Charge-transfer excitons in pentacene:perfluoropentacene co-crystal —
•Ana M. Valencia Garcia[1,2], Darius Günder[3], Michele Guerrini[1,2], Tobias Breuer[3], Gregor Witte[3], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Physics Dept., Humboldt-Universität zu Berlin & IRIS Adlershof — [3]Philipps-Universität Marburg, Molekulare Festkörperphysik, Marburg

Disclosing the nature of optical excitations in organic co-crystals is a challenge due to the complex interplay between the structural arrangement of the molecules and long-range electronic interactions in these systems. For these reasons, the application of isolated cluster models is highly questionable. By means of density functional theory and many-body perturbation theory, we investigate the electronic and optical properties of the triclinic pentacene:perfluoropentacene co-crystal. The band-structure analysis indicates that the highest-occupied and the lowest-unoccupied states are mainly localized on different molecules, suggesting the presence of a charge-transfer exciton at the lowest energy, which is indeed revealed in the dielectric tensor computed from the solution of the Bethe-Salpeter equation. We demonstrate that this feature cannot be reproduced by a molecular cluster model where the first excitation is unambiguously polarized along the short molecular axis. Comparison with corresponding measurements clarifies the importance of adequate periodic treatment of molecular co-crystals to correctly reproduce the character of their excitations [1]. [1] Günder, Valencia, et al., in preparation.

CPP 5.19   Tue 17:30   P

Towards an accurate calculation of excitation energies of Bacteriochlorophyll complexes with Green's function-based many-body perturbation theory —
•Zohreh Hashemi[1] and Linn Leppert[1,2] — [1]Institute of Physics, University of Bayreuth, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

Bacteriochlorophylls (BCL) are a family of chromophores with key functions in the primary energy-converting processes of bacterial photosynthesis. *In vivo*, BCLs are embedded in densely packed pigment-protein complexes; an accurate prediction of their electronic structure and excited states is key to understanding their interactions with each other and with their protein environment. However, the sheer size of these complexes, is presently an insurmountable challenge for highly accurate quantum chemical calculations.

Here we present calculations of the optoelectronic properties of BCL monomers and dimers based on first principles Green's function-based many-body perturbation theory within the GW and Bethe-Salpeter equation (BSE) approach. We find that optical excitations calculated with GW+BSE are in excellent agreement with experimental data and state-of-the-art wavefunction-based approaches - but achieved at considerably lower computational cost than the latter. Our study provides accurate reference results and highlights the potential of the GW+BSE approach for the simulation of larger pigment complexes.

CPP 6: Poster Session II

Complex Fluids and Colloids, Micelles and Vesicles (1-6); Crystallization, Nucleation and Self-Assembly (7-9); Modeling and Simulation of Soft Matter (10-19); Polymer and Molecular Dynamics, Friction and Rheology (20-23); Polymer Networks and Elastomers (24-26).

Time: Tuesday 17:30–19:30   Location: P

CPP 6.1   Tue 17:30   P

Self-assembled micelles in aqueous diblock copolymer solution — •Yanan Li[1], Chia-Hsin Ko[1], Varvara Chrysostomou[2], Dmitry Molodenskiy[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Micelles with stimuli-responsive behavior have attracted great interest as nanocarriers, especially for drug delivery. Here, we investigate the diblock copolymer poly(2-(dimethylamino) ethyl methacrylate)-*b*-poly(lauryl methacrylate) (PDMAEMA-*b*-PLMA), having both pH and thermoresponsive properties in aqueous solution [1]. The self-assembled micelles can be applied in gene transfer and drug delivery applications. We investigate both the pH-dependent micellar structures depending on concentration and the designable micellar shapes from two preparation methods by dynamic light scattering and synchrotron small-angle x-ray scattering. Depending on the preparation method, cylindrical or ellipsoidal micelles are formed. In addition, as the solution is brought from the basic to the acidic state, the micellar size increases, which we attribute to the expansion of the charged PDMAEMA blocks.

[1] V. Chrysostomou, S. Pispas, *J. Polym. Sci. A: Polym. Chem.* **2018**, *56*, 598.

CPP 6.2   Tue 17:30   P

Direct Measurement of the Forces Acting Between Colloidal Silica Particles — •Thomas Tilger, Michael Ludwig, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Natural colloidal dispersions have accompanied mankind in the form of blood or milk ever since. Besides this, artificial systems have gained a significant importance for our daily life during the last decades. From the production of many cosmetics or the water purification and sewage water treatment to the medical field, colloidal systems are widely used nowadays.

For all these applications, it is of special interest to gain an understanding of which interparticle forces govern the stability of colloidal dispersions and how this stability can be tailored. In electrolyte solutions, the classical DLVO theory describes these interactions as a superposition of van der Waals and electrostatic double layer forces. Complex fluids such as micellar dispersions show additional oscillatory contributions caused by a structuring of the micelles.

For a detailed examination of these two regimes, we directly measure the forces between two colloidal silica particles in aqueous solutions by the colloidal probe AFM (atomic force microscopy) technique. Varying the concentration of sodium chloride solutions allows us to compare the transition from the double layer to the van der Waals dominated regime with the predictions of the DLVO theory. Similar measurements for the anionic surfactant sodium dodecyl sulfate (SDS) reveal a structuring of the SDS micelles under confinement.

CPP 6.3   Tue 17:30   P

Aggregation of Gold Nanoparticles: Effects of Ion Type, Salt Concentration, and Aging — •Philipp Ritzert and Regine v. Klitzing — TU Darmstadt, Institute for Condensed Matter Physics, Soft Matter at Interfaces, Hochschulstr. 8, 64283, Darmstadt

The combination of inorganic nanoparticles (NPs) with (responsive) organic polymer matrices advances numerous scientific and technical applications, *e.g.* catalysis, nanoactuation, and medical engineering. Despite considerable progress of embedding NPs into a matrix, the process is often not well-controlled and the composite manufacturing relies on trial-and-error to augment the product quality. Better control over the product manufacturing (*i.e.* NP incorporation) enhances the applicability through more complex NP assemblies.

The project aims at the control of gold NP structuring in a polymer brush matrix. Gold NPs present a versatile model system as they are easily synthesized and stabilized. Furthermore, they exhibit a strong localized surface plasmon resonance in the visible range. Addition of salt triggers the re-ordering, thus, providing multiple adjusting parameters: salt concentration, ion type, and exposure time.

Preceeding composite manufacturing, characterizing the response of gold NPs is essential. The present contribution studies the time evolution of the optical absorption spectra of citrate-capped gold NP suspensions (diameter approx. 13 nm) containing different concentrations of various monovalent sodium salts along the Hofmeister series. In addition, the project exemplifies the influence of basic gold NP properties, namely size and capping molecule.

CPP 6.4   Tue 17:30   P

Mesoscale computer simulations of diffusion and sedimentation of colloidal suspensions — •Yashraj Wani[1], Penelope Grace Kovakas[2], Arash Nikoubashman[1], and Michael Howard[2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [2]Department of Chemical Engineering, Auburn University, Auburn, AL 36849, USA

The diffusive motion in colloidal suspensions is a central process in soft matter, and it also plays an essential role for a wide range of applications. Through simulations, we investigated the self- and collective diffusion in suspensions of spherical colloids at various solute concentrations. To this end, we tested several methods with and without hydrodynamic interactions (HI). We found reasonable agreement for the long-time self-diffusion coefficients between all methods, which is in agreement with previous theoretical considerations. There were, however, fundamental differences in the collective diffusivity (quantified via the sedimentation coefficients) between the various methods: When HI were neglected, the collective diffusivity was identical to the short-time self-diffusion, whereas in the simulations with HI, the sedimentation coefficients decreased with increasing solute concentration. Finally, we applied our methodology to study the equilibrium dynamics of cubic colloids.

CPP 6.5   Tue 17:30   P

Effects of polymer block length asymmetry and temperature on the nanoscale morphology of thermoresponsive double hydrophilic block copolymers in aqueous solutions — •Apostolos Vagias[1], Aris Papagiannopoulos[2], Lucas P. Kreuzer[1], Despoina Giaouzi[2], Sebastian Busch[3], Stergios Pispas[2], and Peter Müller-Buschbaum[1,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [2]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens, Greece — [3]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, 85748 Garching, Germany — [4]Technische Universität München, Physik- Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching, Germany

We combine Fourier transform infrared (FTIR) spectroscopy and small angle neutron scattering (SANS) to identify block length asymmetry and temperature effects on the nanoscale assemblies of novel thermoresponsive double hydrophilic poly(N-isopropylacrylamide)-block-poly(oligo ethylene glycol methyl ether acrylate) (PNIPAM-b-POEGA) diblock copolymers. Morphological transformations from hierarchical assemblies to more well-defined spherical morphologies were identified upon heating. Alteration in the PNIPAM block length induces differences in the strength and/or amount of hydrogen bonding and hydrophobic interactions and molecular solvation.

CPP 6.6   Tue 17:30   P

Rotating spherical particle in a continuous viscoelastic medium — a microrheological example situation — •Sonja K. Richter, Claudius D. Deters, and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

We consider rigid spherical particles in a continuous one-component viscoelastic environment that are subject to an external dynamic torque. A dynamic relaxation parameter quantifies the deformational

memory of the embedding material. Consequently we can interpolate between damped reversible deformation dynamics and net terminal flow of the viscoelastic surroundings using the same formalism [1]. On this basis, we determine the dynamic linear response function for particle rotations that are driven by the external torque under no-slip conditions on the particle surface [2]. Specifically, we derive explicit expressions for the induced deformation and flow fields in the surrounding viscoelastic medium. To link to magnetic microrheology, we address magnetically anisotropic particles that are driven by a dynamic external magnetic field. Corresponding magnetic susceptibility functions are evaluated [2]. Overall, we expect that our results will be important in the context of microrheological measurements on soft and biological visoelastic matter.

[1] M. Puljiz, A. M. Menzel, *Phys. Rev. E* **99**, 012601 (2019).
[2] S. K. Richter, C. D. Deters, A. M. Menzel, *EPL (Europhys. Lett.)*, accepted.

CPP 6.7   Tue 17:30   P

STM and DFT study of BF4 anion migration on a triaza-triangulenium SAM on Au(111) — •Sᴇʀɢɪɪ Sɴᴇɢɪʀ[1], Yᴀɴɴɪᴄᴋ Dᴀᴘᴘᴇ[2], Dᴍʏᴛʀᴏ Sʏsᴏɪᴇᴠ[3], Oʟɪᴠɪᴇʀ Pʟᴜᴄʜᴇʀʏ[4], Tʜᴏᴍᴀs Hᴜʜɴ[1], and Eʟᴋᴇ Sᴄʜᴇᴇʀ[1] — [1]University of Konstanz, Konstanz, Germany — [2]SPEC, University Paris-Saclay, France — [3]I. Org. Chem. & Biochem., Prague — [4]INSP, Sorbonne University, France

Chemical coupling of functional molecules with so-called platforms allows the formation of functional Self-Assembled Monolayer (SAM). An example is triazatriangulenium (TATA), with an extended aromatic core, allowing the formation of good electronic contact with the metal surface. Here we present studies on SAMs of TATA-BF4 molecules on Au(111) by means of Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT). In solution, these molecules exist as ion pairs of TATA+ and BF4-. However, under electrochemical deposition on Au(111), on the TATA+ cations formed SAMs the BF4-anions seemingly disappear. Our STM experiments reveal dissociation of the TATA-BF4 complex1. The TATA+ remains stable within the SAM while the BF4- spontaneously migrates through the TATA SAM on the surface. DFT calculations show a reduction of the TATA-BF4 binding energy after deposition. 1.S.Snegir, Y. J.Dappe, D.Sysoiev, O.Pluchery, T.Huhn, E.Scheer, PCCP 2021, 23, 9930 - 9937.

CPP 6.8   Tue 17:30   P

Ordering of small polymer systems through the prism of partition function zeros. — •Tɪᴍᴜʀ Sʜᴀᴋɪʀᴏᴠ and Wᴏʟғɢᴀɴɢ Pᴀᴜʟ — Institute of Physics, University of Halle, Halle, Germany

Typical low temperature conformations of small alkane systems (single chains and few chain aggregates) differ frequently from the melt ones: even relatively short chains are folded in non-trivial structures at low temperatures [1]. The ordering of a system is related to change of thermodynamic and conformational characteristics of chains. In the case of big systems, the changes occur at one the same transition temperature, whereas for small systems the typical temperatures of the changes can be shifted relative to each other. The sensitivity of thermodynamic functions to the shift differs and can be hidden because of a widening of the transition region of the small system. We present here the results of an analysis of the partition function zeros, which helps to identify a two stage conformational reorganization of small alkane systems. Our calculations are based on Wang-Landau-type Monte Carlo simulations [2,3] of a chemically realistic united atom model [4].

[1] T. Shakirov, and W. Paul, J. Chem. Phys. 2019, 150, 084903.
[2] F. Liang, C. Liu, R. J Carroll, J. Am. Stat. Assoc. 2007, 102, 305-320.
[3] T. Shakirov, Comp. Phys. Commun. 228 (2018): 38-43.
[4] W. Paul, D. Y. Yoon, and G. D. Smith, J. Chem. Phys. 103 (1995) 1702-1709.

CPP 6.9   Tue 17:30   P

Alteration of self-assembly monolayers and their interactions with zinc oxide surfaces: A DFT study — •Aᴢᴀᴅᴇ YᴀᴢᴅᴀɴYᴀʀ[1], Pᴇᴛɪᴀ Aᴛᴀɴᴀsᴏᴠᴀ[2], and Mᴀʀɪᴀ Fʏᴛᴀ[1] — [1]Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute for Materials Science, Bioinspired Materials, Heisenbergstr. 3, 70569 Stuttgart, Germany

Self-assembled monolayers (SAMs) have gained profound interest due to their broad range of applicability such as in molecular electronics, bio-sensing and heterogeneous catalysis. One of the advantages of SAMs is the feasibility they provide in altering and controlling the properties of the substrate. Here, we use Density Functional Theory

(DFT) to study the influence of various variations on the SAM-zinc oxide surface interactions. Specifically, we study the effect of several head groups (thiol, silane, phosphonate) and various crystallographic planes. We limit our work to SAMs of three methylene groups (CH2) in the chain with an azide functional group. The energetics of the system will be determined and compared in order to understand the strength of the SAM-surface interaction, which we expect to be greatly impacted by the type of the head group of the SAMs. We will also provide details on the specific interaction sites of the head group with the surface and the electronic structure. We discuss the relevance of these materials as functionalized templates for novel applications in catalysis and sensing.

CPP 6.10   Tue 17:30   P

Dissipative Self-Organization of Interfaces and Membranes — •Gʀᴇɢᴏʀ Iʙʙᴇᴋᴇɴ and Mᴀʀᴄᴜs Müʟʟᴇʀ — Frierich-Hund-Platz 1, 37075 Göttingen

Coupling a self-assembling system to a reaction cycle, we go beyond equilibrium self-assembly toward systems that dissipate energy and thus exhibit new, unique features of dynamic self-organization. We consider the general case of a precursor reacting with a fuel to a product, which itself can decay back to the precursor. To do so, a continuum model is utilized that treats concentrations as order parameters. Within the model, the free energy is given as a functional of the concentrations and the dynamics are computed via the chemical potentials. We show that under the assumption that the fuel diffuses faster than the reacting polymers, reactions introduce an effective connectivity between precursor and product. This way the systems show entirely different features than their respective equilibrium counterpart. For instance, a homopolymer melt can form lamellae, cylinders, spheres, as well as networks, similar to a diblock copolymer melt, and a solution with two reacting homopolymers can form bilayers. The length scale of emergent structures depends on the reaction rates. This way, one can control the size of micelles and vesicles in solution, by coupling an amphiphilic diblock copolymer to a hydrophilic precursor, giving rise to an interplay between the architecture- and the reaction-rate-determined length scales.

CPP 6.11   Tue 17:30   P

Measuring the line tension of a hemifusion diaphragm — •Yu-Jᴜɴɢ Sᴜ, Yᴜʟɪʏᴀ Sᴍɪʀɴᴏᴠᴀ, and Mᴀʀᴄᴜs Müʟʟᴇʀ — Institut für Theoretische Physik, Georg-August-Universität, 37077 Göttingen, Deutschland

Changes of membrane topology are essential to cellular transport processes, such as e.g., synaptic release. The molecular pathways, however, are only incompletely understood. The hemifusion diaphragm (HD) is a putative intermediate, where two apposing membranes are locally fused into a single-membrane patch. The line tension of the three-bilayer junction at the rim of the HD controls the size and stability of the HD, and it is an important parameter for phenomenological free-energy models of fusion and fission processes. In the canonical ensemble, where the number of lipids is fixed, the line tension, λ, of the HD, which tends to decrease the area of the HD, is balanced by the membrane tension, π, resulting in a two-dimensional analog of the Laplace equation between λ, π, and the radius, R, of the HD. Using molecular dynamics simulation of the coarse-grained MARTINI model, we study this free-energy balance and calculate the line tension as a function of the membrane tension or the distance between the flat membranes in apposition. The results are compared to alternate estimates, e.g., obtained from the shape fluctuations of the rim of the HD.

CPP 6.12   Tue 17:30   P

Stability of the hemifusion diaphragm and the rim pore — •Yᴜʟɪʏᴀ Sᴍɪʀɴᴏᴠᴀ and Mᴀʀᴄᴜs Müʟʟᴇʀ — Institute for Theoretical Physics, Georg-August University, Göttingen, Germany

Synaptic transmission is a fundamental biophysical process that involves the exocytosis (neurotransmitter release) and endocytosis (vesicle recovery) of small synaptic vesicles at the presynaptic plasma membrane. Whereas the molecular mechanisms of these topology-altering membrane processes are only incompletely understood, it is hypothesized that a hemifusion diaphragm (HD), i.e., an extended single-membrane-thick, lipidic connection between the two apposing membranes, is an important intermediate state. We develop a phenomenological model to investigate the free-energy landscape of a HD with a (rim) pore (RP) that is formed inside the HD and borders the three-bilayer junction at the HD's rim. In the limit that the RP attains the

size of the HD, a complete fusion pore is formed. In the absence of the RP, HDs of different sizes are (meta)stable in the canonical ensemble. It appears, however, to be difficult to stabilize a HD+RP complex in the canonical ensemble. Membrane tension, intermembrane distance, and the line tensions of a membrane pore, a HD, and a fusion pore, as well as external control of the HD's size are important parameters that dictate the (meta)stability of the HD+RP complex and, thereby, the pathway of synaptic transmission.

CPP 6.13   Tue 17:30   P

Analytical and computational study of advection-diffusion-reaction processes in catalytic fibrous membranes — •Gabriel Sitaru and Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

We investigate the efficiency of multi-step catalytic systems where a reactant species is flown through a set of fibrous catalytic membranes. The complexity of such systems arises from the interplay of three different time scales: advection, diffusion and reaction. A theory based on infinitely long cylindrical catalytic sites is developed for the steady-state of an advection-diffusion limited reaction. Additionally, the time-dependent concentration profiles are computed using a Lattice-Boltzmann based solver for both the advection-diffusion-reaction and the Navier-Stokes equations. The comparison shows a good agreement between the theory and the numerical results in the intermediate and high Péclet regimes. Both methods can be easily used to predict the efficiency of a multi-step catalysis in fibrous membranes with various geometries.

CPP 6.14   Tue 17:30   P

BoltzmaNN: Predicting effective pair potentials and equations of state using neural networks — •Fabian Berressem and Arash Nikoubashman — Johannes Gutenberg University, Mainz

Neural networks (NNs) are employed to predict equations of state from a given isotropic pair potential using the virial expansion of the pressure. The NNs are trained with data from molecular dynamics simulations of monoatomic gases and liquids, sampled in the NVT ensemble at various densities. We find that the NNs provide much more accurate results compared to the analytic low-density limit estimate of the second virial coefficient and the Carnahan-Starling equation of state for hard sphere liquids. Furthermore, we design and train NNs for computing (effective) pair potentials from radial pair distribution functions, $g(r)$, a task that is often performed for inverse design and coarse-graining. Providing the NNs with additional information on the forces greatly improves the accuracy of the predictions since more correlations are taken into account; the predicted potentials become smoother, are significantly closer to the target potentials, and are more transferable as a result.

CPP 6.15   Tue 17:30   P

Establishment of a workflow and comparison of scattering data driven molecular dynamics simulations for two water models — •Veronika Reich[1], Sebastian Busch[1], and Martin Müller[2] — [1]German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ), Helmholtz-Zentrum Hereon, Lichtenbergstr. 1, 85748 Garching bei München, Germany — [2]Institute of Materials Physics, Helmholtz-Zentrum Hereon, German Engineering Materials Science Centre (GEMS) and Heinz Maier-Leibnitz Zentrum (MLZ)

Molecular dynamics simulations are increasingly used to evaluate scattering data. For many systems, reliable force fields are available that yield simulations which are compatible with the measured data. For many other systems, however, the agreement between simulation and experiment is not satisfactory yet. In this work, we aim to couple measured and simulated data on the example of different liquid water models in order to optimize force fields.

Two water models, TIP3P and TIP4P/2005, were first simulated by molecular dynamics simulations with the program LAMMPS and further the program SASSENA was used to calculate the corresponding scattering signals. The outcomes were compared to already existing experimental data and changes in the underlying force fields where evaluated in terms of their impact on the behaviour of the simulation.

CPP 6.16   Tue 17:30   P

Ground- and excited-state properties of tetraphenyl compounds from first-principles calculations — •Kevin Eberheim, Christof Dues, and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität

Gießen, 35392 Gießen, Germany

Tetraphenyl compounds with formula $X(C_6H_5)_4$ (X being a tetravalent atom of the 14_{th} group such as C, Si, Ge, Sn, Pb), crystallize either in a tetragonal crystalline structure or in an amorph phase [1]. Depending on their habitus, the compounds are characterized by very different optical properties. The molecular crystals are known for their second harmonic generation (SHG) properties, while the amorph phase is a white light emitter. Tetraphenyl molecules feature indeed the delocalized π-orbitals, which have been proposed as a prerequisite for the white-light generation [2]. In an attempt to understand the mechanisms related to the white light emission, we model the structural, electronic and vibrational properties of different $X(C_6H_5)_4$ structures within density functional theory. The calculated structural parameters closely reproduce the measured values, however vdW corrections are crucial for a correct description of the structural properties. This confirms that dispersion forces are responsible for the intermolecular bonds in the compound. Different implementations of the vdW forces lead to very similar results. Calculated vibrational properties are in agreement with measured Raman spectra. [1] A Kitaigorodsky, Molecular crystals and Molecules, Acad. Press (1973). [2] Nils W. Rosemann et al., J. Am. Chem. Soc. 138, 16224 (2016), Science 352, 1301 (2016).

CPP 6.17   Tue 17:30   P

Polymer Architectures by Chain Walking Catalysis - Topological Transition From Linear Chains to Dendrimers — •Ron Dockhorn[1], Laura Plüschke[1], Albena Lederer[1], Jan Merna[3], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden, Germany — [2]Technische Universität Dresden, Institute for Theoretical Physics, D-01069 Dresden, Germany — [3]University of Chemistry and Technology Prague, CZ-16628 Praha, Czech Republic

Chain walking (CW) catalysis is a unique approach to synthesize dendritic polyethylenes by a "walking" Pd-α-diimine catalyst into a variety of complex branch-on-branch architectures. Coarse-grained Monte Carlo simulations utilizing the bond fluctuation model of the CW process are performed to investigate the influence of the walking mechanism on the polymer topology. Two distinct regimes can be identified: For low walking rates the structure growths with linear chain extension and low amounts of side chains, whereas high walking rates promote random and isotropic dendritic growth of the molecule. The transition regime is characterized by large amount of branched side chains reflecting a cross-over regime with characteristics of disordered dendronized bottle-brushes controllable by the walking rate of the catalyst. SANS experiments of the CW-polymerized ethylenes are compared to simulation data verifying the observed macro-conformational transitions. The CW one-pot preparation setup tunable by external parameters provides a powerful synthesis route to create dendrigrafts / dendronized polymers.

CPP 6.18   Tue 17:30   P

Aggregation of several flexible-semiflexible block-copolymer chains: flat histogram Monte Carlo simulation — •Viktor Ivanov[1,2], Ekaterina Kruglova[2], Julia Martemyanova[2], Timur Shakirov[1], and Wolfgang Paul[1] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany — [2]Lomonosov Moscow State University, Faculty of Physics, 119992 Moscow, Russia

We study conformational properties of a single multi-block copolymer chain consisting of flexible (F) and semi-flexible (S) blocks with equal composition of F- and S-units and with different affinity to a solvent, as well as the aggregation of several such chains. We perform flat histogram Monte Carlo simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm. We use the two-dimensional density of states, which depends on the energy of intramolecular stiffness and on the energy of non-valence interactions. We present data on different non-trivial globular morphologies, including several structures with high orientational ordering of bonds. Pseudo-phase diagrams in variables temperature vs. stiffness parameter are presented for different values of the block length. We also present our recent results on the aggregation behaviour of several FS-block-copolymer chains and discuss the possibility of shape-persistent aggregation of globules. We acknowledge the financial support from RFBR (grant 19-53-12006-NNIO-a) and DFG (project PA 473/18-1) and thank Moscow State University Supercomputer Center for providing the computational resources.

CPP 6.19   Tue 17:30   P

Crystallization of oligomers in melts between two hard walls: flat histogram Monte Carlo simulation — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany

We study conformational properties of short polymer chains in melts between two hard walls. Our final goal is to reveal physical factors which are responsible for a particular scenario of surface-induced polymer crystallization (e.g., the nucleation and growth or the 1st order prefreezing). We use a coarse-grained model and perform flat histogram Monte Carlo (MC) simulations based on the stochastic approximation Monte Carlo (SAMC) algorithm. We analyse different order parameters: nematic orientational order parameter, bond orientation order parameters (Steinhardt parameters), hexagonal order parameter (which shows a quasi-two-dimensional stacking of chain cross sections in a plane perpendicular to the director). We see the nematic transition (formation of rotator phase) upon cooling, followed by a crystallization transition. We are able to observe a coexistence of an isotopic structure in the center of the film with ordered structures at the walls at intermediate values of energies (in microcanonical analysis). We are able to localise the transition points between different pseudo-phases quite precisely. Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

CPP 6.20 Tue 17:30 P
Pressure and temperature-dependent changes in the microstructure of linear mono-ols — •Jennifer Bolle[1], Alexander Faulstich[1], Martina Požar[2], Aurélien Perera[3], Michael Paulus[1], Metin Tolan[1], and Christian Sternemann[1] — [1]Fakultät für Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]University of Split, Faculty of Science, Rudera Boškovića 33, 21000, Split, Croatia — [3]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, 4 Place Jussieu, F75252, Paris. cedex 05, France

Hydrogen bonds are essential for understanding the microscopic structure of water, aqueous solutions and associated fluids in general. They stabilize the structure of peptides and proteins and are the driving force for association in molecular fluids. In this study, the evolution of the microstructure of a series of linear monohydroxy alcohols (mono-ols) with temperature and pressure was investigated by X-ray diffraction at beamlines BL2 and BL9 of the synchrotron radiation source DELTA (TU-Dortmund, Germany). Comparing the behavior of the so-called pre-peak in the diffraction patterns of the mono-ols with increasing chain length, the influence of steric hindrance on the charge order of these liquids was systematically studied. The results are compared with calculated diffraction intensities based on molecular dynamics simulations and interpreted on the basis of changes in their microstructure. We observe that the charge order for all the studied alcohols is significantly affected by pressure and temperature and strongly depends on chain length.

CPP 6.21 Tue 17:30 P
Systematic derivation of hydrodynamic equations for viscoelastic phase separation — •Burkhard Duenweg[1], Dominic Spiller[1], Maria Lukacova[2], Aaron Brunk[2], Herbert Egger[3], and Oliver Habrich[3] — [1]MPI for Polymer Research Mainz — [2]Mathematics, JGU Mainz — [3]Mathematics, TU Darmstadt

We present a simple hydrodynamic two-fluid model aiming at the description of the phase separation of polymer solutions with viscoelastic effects. It is directly based upon the coarse-graining of a molecular model (such that all degrees of freedom have a clear molecular interpretation), and a free-energy functional. The dynamics is split into a conservative and a dissipative part, following the GENERIC formalism. In a first step, we derive an extended model where inertial dynamics of the macromolecules and of the relative motion of the two fluids is taken into account. In the second step, we eliminate these inertial contributions and, as a replacement, introduce phenomenological dissipative terms. The final simplified model is similar, though not identical, to models that have been discussed previously. In contrast to the traditional two-scale description that is used to derive rheological equations of motion, we here treat the hydrodynamic and the macromolecular degrees of freedom on the same basis. Notably, we find a rheological constitutive equation that differs from the standard Oldroyd-B model. This difference may be traced back to a different underlying statistical-mechanical ensemble that is used for averaging the stress.

CPP 6.22 Tue 17:30 P
Controlling the dynamics of soft, coarse-grained polymer fluids at surfaces — •Pritam Kumar Jana[1], Petra Bacova[2], Ludwig Schneider[1], Vangelis Harmandaris[2], Patrycja Polinska[3], Craig Burkhard[4], and Marcus Müller[1] — [1]Institute for Theoretical Physics, University of Goettingen — [2]Institute of Applied and Computational Mathematics, Foundation for Research and Technology-Hellas, Heraklion, Greece — [3]Goodyear S.A., Colmar-Berg L-7750, Luxembourg — [4]The Goodyear Tire and Rubber Company, Akron, Ohio 44305, United States

The rheological properties of composites derived from fillers in a polymer matrix depend on particle size, filler loading, and dispersion, as well as the interfacial interaction between the fillers and polymer matrix. For the coarse-grained modeling of such systems, it is crucial to pay attention to the fluid flow past the solid filler surface because the classical no-slip hydrodynamic boundary condition does not hold on the micro-and nanoscopic length scale. Instead, the flow is characterized by a microscopically small but finite slip length. To explore the dynamics and slippage, we perform both atomistic and highly coarse-grained (hCG) simulations. In the atomistic simulations, we study the dynamics of polybutadiene close to a silica surface. In the hCG scale, since the solid surface appears smooth, special simulation techniques are required to generate friction at the solid-fluid contact and control slippage. We devise a simulation strategy that can reproduce the dynamics of the polymers close to the wall as seen in the atomistic simulations. The parametrized hCG model, which is devised by comparison with the atomistic simulations, allows the exploration of the dynamics and slippage of polymers with a wide range of molecular weights.

CPP 6.23 Tue 17:30 P
Molecular origins of shear-thinning in polymer melts — •Ranajay Datta, Friederike Schmid, and Peter Virnau — Institute of Physics, Johannes Gutenberg University, Staudingerweg 9, 55128 Mainz, Germany

We investigate the molecular origin of shear-thinning in melts of flexible, semiflexible and rigid oligomers with coarse-grained simulations of a sheared melt [1]. Emergence of entanglements and nematic phases in equilibrium, alignment, stretching and tumbling modes or suppression of the latter all contribute to understanding how macroscopic flow properties emerge from the molecular level. By performing simulations of single chains in shear flow, we identify which of these phenomena are of collective nature and arise through interchain interactions and which are already present in dilute systems.

Reference:
[1] https://arxiv.org/abs/2101.03645v2

CPP 6.24 Tue 17:30 P
Phase behavior of randomly crosslinked diblock copolymers — •Gaoyuan Wang, Annette Zippelius, and Marcus Müller — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Deutschland

We have investigated the structure and the phase behavior of randomly crosslinked polymer networks formed by connecting symmetric diblock copolymers via covalent bonds. Particle-base Monte-Carlo simulation is applied to study the order-disorder transition, controlled by the Flory-Huggins parameter χ. We provide an accurate phase diagram, in which the $\chi_c N$ of the ODT is shown as a function of the crosslink density p and Flory-Huggins parameter of the preparation state $\chi_p N$. Depending on $\chi_p N$, the random crosslinks support the disordered or periodically ordered state over a larger range of incompatibilities (χN), because the irreversible bonds impart a memory of the structure that existed at their formation. Knowing the amount of crosslinking required to retain a microphase-separated or disordered structure at a χN that considerably differs from the preparation state is helpful for generating desired states, which may only be metastable without crosslinks.

CPP 6.25 Tue 17:30 P
Understanding the structure of reversible networks made of star polymers — •Kiran Suresh Kumar[1,2], Toni Müller[1,2], Jens-Uwe Sommer[1,2], and Michael Lang[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Institut Theorie der Polymere, Hohe Strasse 6, 01069 Dresden, Germany — [2]Institute für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

Bonds in reversible networks break and form continuously allowing the material to flow and self-heal on long time scales while being a solid on short times. Recent work utilized a regular star branched architecture in combination with a controlled pairwise association of reversible groups to reveal the impact of network defects on the material properties [1-4]. We develop a model for network structure by combining previous work on network defects in irreversible networks [5] with the method of balance equations [6] for reversible systems. The model predictions for the frequency of different star types are tested by Monte Carlo simulations of network structure.

[1] Rossow, T.; Habicht, A.; Seiffert, S. Macromolecules 2014, 51, 6473-6482. [2] Tang, S.; Wang, M.; Olsen , B. D. J. Am. Chem. Soc. 2015, 137, 3946-3957. [3] Tang, S.; Habicht, A.; Li, S.; Seiffert, S.; Olsen, B. D. Macromolecules 2016, 49, 5599-5608. [4] Ramirez, J.; Dursch, T. J.; Olsen , B. D. Macromolecules 2018, 51, 2517-2525. [5] Lang, M.; Schwenke, K.; Sommer, J.-U. Macromolecules 2012, 45, 4886- 4895. [6] Lang, M.; Kumar, K. S. Macromolecules 2021, 10.1021/acs.macromol.1c00718.

CPP 6.26   Tue 17:30   P
Thermal transport of epoxy networks: Bond engineering and network microstructures — •Manjesh Kumar Singh[1] and Debashish Mukherji[2] — [1]Department of Mechanical Engineering, Indian Institute of Technology Kanpur, Kanpur: 208016, Uttar Pradesh, India — [2]Quantum Matter Institute, University of British Columbia, Vancouver BC V6T 1Z4, Canada

Thermal transport coefficient (k) is a central property of condensed matter systems, where establishing the molecular level understanding is extremely important to tailor the materials properties for their possible uses under extreme environmental and practical conditions. Here polymers are an important class of materials because they provide different pathways for the energy transfer. For example, the heat flow between the two covalently bonded monomers is over 100 times faster than between the two non-bonded monomers [1]. Therefore, the delicate balance between these two contributions often provides a guiding tool for the design of tailor made polymeric materials with extraordinary thermal properties. Traditionally most studies have investigated k in the linear polymeric materials, the recent interests have also been directed towards the epoxy network. Using molecular dynamics simulations, we investigate the factors effecting k of epoxy networks. We emphasize on the importance of the bond types and their influence on the network microstructures, with a goal to provide a guiding principle for the tunability in k [2].

[1] Bhardwaj et al., ACS Nano 15, 1826 (2021). [2] Mukherji et al., Physical Review Materials 5, 025602 (2021).

CPP 7: Soft Matter (joint session CPP/DY)

Time: Wednesday 10:00–12:45   Location: H3

Invited Talk   CPP 7.1   Wed 10:00   H3
Chemically Fueled Out-Of-Equilibrium Self-Assemblies and Autonomous Material Systems — •Andreas Walther — Department of Chemistry, University of Mainz

Living self-organizing systems operate far-from-equilibrium and maintain functions by constant energy dissipation in feedback-regulated adaptive steady states. In stark contrast, man made self-assemblies are typically oriented towards equilibrium or deep metastable states.

Some of the next steps in self-assembling systems are to approach multicomponent co-assembling systems, and to master temporal behavior as well as complex adaptation mechanisms. The latter require new types of internal control mechanisms, such as kinetic control over opposing reactions (built-up/destruction), the integration of feedback mechanisms, or the use of energy dissipation to sustain structures only as long as a chemical fuel is available. This ultimately goes along with a transition towards out-of-equilibrium complex systems, in which multiple components self-assemble dynamically in a non-linear and adaptive fashion.

In this talk I will present two conceptual pathways towards out-of-equilibrium systems, (i) driven environments and (ii) driven structures, which allow to program self-assemblies and materials with lifetimes and programmable steady state dynamics using feedback mechanisms and conversion dynamics of chemical fuels. This will be showcased for different self-assembling systems (polymers, peptides, DNA), and the connection to hydrogels and photonic materials demonstrates possibilities for new horizons in materials science.

CPP 7.2   Wed 10:30   H3
UV-light printing on APTES functionalized SiO2 surfaces: New approach for nanoparticle assembly — •Sergii Snegir[1], Olivier Plichery[2], Thomas Huhn[1], and Elke Scheer[1] — [1]University of Konstanz, Konstanz, Germany — [2]INSP, Sorbonne University, France

The 3-Aminopropyl)trimethoxysilane (APTES) terminated SiO2 surface allows creating self-assembled monolayers (SAMs) of gold nanoparticles (AuNPs). However, further functionalization of AuNPs with thiol-containing molecules leads to their strong aggregation due to the appearance of uncompensated dipole moments on the AuNP. Therefore, we developed a UV-light fixation method, which anchors AuNPs on their initial positions on the APTES surface prior to the process of AuNP functionalization. Herein, we present detailed studies of the passivation efficiency as the function of UV light wavelength, time of exposure, the concentration of O2, N2, O3 gases (1). We have found that the combination of O3 and UV light under ambient atmospheric conditions lead to complete passivation of APTES terminated glass already after 2 min of UV exposure (26.1 mW/cm2). We have tested also the possibility to use the UV-light passivation for printing on APTES terminated surfaces by using different chromium masks. With this method, we can create SAMs of AuNP with different geometry and size (resolution limit several um) on a SiO2 surface (glass/quartz/silicon). 1. S.Snegir, T.Huhn,J. Boneberg, S.Haus, O.Pluchery, E.Scheer, J.Phys.Chem.C, 2020,124(35), 19259-19266.

CPP 7.3   Wed 10:45   H3
In situ GISAXS analysis of printed hybrid diblock copolymer thin films containing mixed magnetic nanoparticles — •Christopher Everett[1], Xinyu Jiang[1], Manuel Scheel[1], Huaying Zhong[1], Martin Bitsch[2], Martina Plank[3], Markus Gallei[2], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, Garching, Germany — [2]Saarland University, LS Polymer Chemistry, Saarbrücken, Germany — [3]TU Darmstadt, Ernst-Berl-Institut, Darmstadt, Germany — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [5]KTH Royal Institute of Technology, Stockholm, Sweden — [6]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Garching, Germany

Diblock copolymer (DBC) thin films that form periodic nanostructures are appropriate scaffolds for magnetic nanoparticles (NPs) and have potential for a variety of applications such as highly functional magnetic sensors and in high-density magnetic data storage. In this investigation, ultra-high molecular weight PS-b-PMMA films are used as templates for both ferrimagnetic magnetite NP and ferromagnetic Ni NPs. The thin films, containing up to 6 wt% NPs, are fabricated by a slot-die coating technique and the morphological evolution of the films during the deposition and drying process is monitored in situ with grazing incidence small-angle X-ray scattering (GISAXS). The dry thin films are subjected to solvent vapor annealing and ordered nanostructured hybrid films are obtained. Using a SQUID magnetometer, the resulting magnetic properties are measured.

15 min. break

Invited Talk   CPP 7.4   Wed 11:15   H3
The quest for robust superhydrophobic surfaces — •Robin Ras — Department of Applied Physics, Aalto University, Espoo, Finland

Nature offers various examples of extreme water-repellency, such as the leaves of Lotus plant and wings of cicada. The water repellency allows plants for efficient photosynthesis even in dusty environments, and allows large-wing insects to fly even in humid conditions. Likewise, our technological society could benefit from surfaces that stay clean and dry in challenging conditions. For example, solar cells on roof tops loose efficiency when they are covered with sand and dust.

The extreme water-repellency, also called superhydrophobicity, is attributed to the combination of micro/nanoscale topography and hy-

drophobic surface chemistry that allows trapping of a thin air film between the water and the solid substrate. The air film effectively shields the water from the solid by reducing the contact area, leading to very high contact angle and very low adhesion and friction. The required topography, however, also makes these surfaces very fragile.

Here I will present the progress made during previous decade, including different strategies for enhancing the mechanical durability. Recently, in collaboration with the group of Xu Deng, we developed an extremely durable superhydrophobic surface, by making use of a microstructured armor that protects the otherwise fragile nanostructures. I will present the concept, and steps that we are taking towards commercialization.

CPP 7.5   Wed 11:45   H3

Calculating Magnetization Fields in Magnetoactive Elastomers: A Cascading Mean-Field Approach — •Dirk Romeis and Marina Saphiannikova — Leibniz Institute of Polymer Research Dresden, Germany

We consider the application of an external magnetic field to a composite of a non-magnetizable elastomer matrix with embedded magnetizable particle inclusions. The resulting interactions are determined by the magnetization field which is generated not only by the external magnetic field but also by the magnetic fields arising due to surrounding inclusions. A comprehensive description requires knowledge about the magnetization of individual particles and of macroscopic portions of the composite. Accordingly, a precise calculation becomes elaborate for a specimen comprising billions of particles. We present a greatly simplified, but accurate approximation for the computation of magnetization fields in such composites. Based on the dipole model, we introduce the cascading mean-field description [1] by separating the magnetization field into three contributions on the micro-, meso-, and macroscale. It is revealed that the contributions are nested into each other, as in the Matryoshka's toy. Our description allows for an efficient and transparent analysis of such composite materials under rather general conditions.

Financial support by DFG, SPP 1713, is gratefully acknowledged.

[1] D. Romeis and M. Saphiannikova: A cascading mean-field approach to the calculation of magnetization fields in magnetoactive elastomers. Polymers, 13(9):1372, 2021.

CPP 7.6   Wed 12:00   H3

Magnetostrictive effects in soft magnetic gels and elastomers — •Lukas Fischer and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Our work focuses on magnetic gels and elastomers, also known as magnetorheological elastomers or ferrogels, that feature a soft elastic matrix enclosing magnetizable particles. These materials react to an applied external magnetic field mainly in a twofold manner: by changing their overall mechanical properties (magnetorheological effect) and by overall macroscopic deformations (magnetostriction).

We have developed a mesoscopic theory to describe the latter effect. For this purpose, we analytically solve the linear elastic problem, linking the particle scale to the scale of overall deformation. To adjust the deformational response, we modify the initial positioning of the particles inside the material, relative to the magnetic field direction [1].

Specific spatial arrangements of the magnetizable particles inside the elastic medium favor specific magnetostrictive modes of deforma-

tion, for example torsion [2]. Targeted modification of the particle size can likewise serve to adjust the magnetostrictive response [3]. Our work supports the construction of magnetically controlled soft actuators that are tailored to requested deformational tasks.

[1] L. Fischer, A. M. Menzel, *J. Chem. Phys.* **151**, 114906 (2019).
[2] L. Fischer, A. M. Menzel, *Phys. Rev. Research* **2**, 023383 (2020).
[3] L. Fischer, A. M. Menzel, *Smart Mater. Struct.* **30**, 014003 (2021).

CPP 7.7   Wed 12:15   H3

Perturbed Jamming transitions — Moumita Maiti[1] and •Michael Schmiedeberg[2] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Theoretische Physik 1, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

By minimizing the interaction energy in a soft sphere system without crossing energy barriers the discontinuous athermal jamming transion can be observed at a packing fraction of about 0.64 in 3D [1]. However, if perturbations like thermal fluctuations [2] or an active self-propulsion [3] are added, the transition becomes continuous and the transition packing fraction might occur at a different density. For example, in case of thermal fluctuations, the transition packing fraction approaches 0.55 in case of small thermal fluctuations [2]. We show that the thermal jamming transition lies within the universality class of directed percolation. As a consequence, athermal jamming is a (singular) limit of a much wider class of perturbed jamming transitions that can also be understood as dynamical transitions [2,4]. Therefore, perturbed jamming transitions open up a large variety of amorphous packings and insights how these packings are related to glassy dynamics.

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002), Phys. Rev. E 68, 011306 (2003).
[2] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018).
[3] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).
[4] L. Milz and M. Schmiedeberg, Phys. Rev. E 88, 062308 (2013); S. Wilken et al., Phys. Rev. Lett. 127, 038002 (2021).

CPP 7.8   Wed 12:30   H3

Fluidity models for amorphous glassy materials — •Robin Lautenschlager and Thomas Voigtmann — Institut für Materialphysik im Weltraum, Deutsches Zentrum für Luft- und Raumfahrt (DLR), 51170 Köln

Different rheological models are proposed to describe the complex flow properties of amorphous glassy materials, such as granular materials or colloidal glasses, intermediate between a solid and liquid behavior. These systems show a strong non-linearity due to stresses and strain rates, as well as time-dependent ageing effects. The materials are hence described by a time-dependent local fluidity as a main rheological quantity. Spatial non-localities are quantified by a characteristic cooperativity length that describes the extent over which neighboring material regions influence their flow behavior.

We compare three different approaches of such fluidity models and discuss their key features regarding the complex flow properties and how they try to reproduce the time-dependent effects of such a flow. We probe the models in a pressure driven two-dimensional-channel-flow and compare their long-time numerical results to analytically estimated steady state solutions for this test case. We will discuss how the models respond to different flow properties to evaluate their usability in applications.

CPP 8: Poster Session III

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

Time: Wednesday 17:30–19:30 Location: P

CPP 8.1 Wed 17:30 P

Janus Particles Self-Assembly: Magnetic and Catalytic Propulsion of Clustered Janus Particles — •Yara Alsaadawi[1], Anna Eichler-Volf[1], Michael Heigl[2], Peter Zahn[1], Manfred Albrecht[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

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

CPP 8.2 Wed 17:30 P

Analytical study of active semiflexible ring polymer — •Christian Anton Philipps, Roland Georg Winkler, and Gerhard Gompper — Forschungszentrum Jülich Institute of Biological Information Processing, Jülich, Germany

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

CPP 8.3 Wed 17:30 P

Predicting the bulk modulus of single-layer 2D COFs from their molecular building-blocks properties — •Antonios Raptakis[1,2], Alexander Croy[1], Arezoo Dianat[1], Rafael Gutierrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str.

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

on the properties of the monomeric units.

CPP 8.4 Wed 17:30 P

The possibilty of spray coating of lignin and characterization of the thin film — •Sophie Snoke[1,2,3], Constantin Harder[1,4], Wienke Reynolds[2], and Stephan V. Roth[1,5] — [1]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [2]Lignopure GmbH, 21073 Hamburg — [3]Institute of Thermal Separation Processes, Technische Universität Hamburg-Harburg, 21073, Hamburg, Germany — [4]Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — [5]KTH Royal Institute of Technology, 100 44 Stockholm, Sweden

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

CPP 8.5 Wed 17:30 P

Inorganic-organic hybrid nanostructures based on biopolymer templating — •Linus Fidelis Huber and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

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

CPP 8.6 Wed 17:30 P

Protein-polysaccharide nanoparticles stabilized by thermal treatment — •Johannes Allwang[1], Yanan Li[1], Stefano Da Vela[2], Dimitris Selianitis[3], Angeliki Chroni[3], Aristeidis Papagiannopoulos[3], and Christine M. Papadakis[1] — [1]Physics Department, Technica University Munich, Garching, Germany — [2]EMBL, DESY, Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

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

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

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

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

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

CPP 8.7 Wed 17:30 P

Colloidal layer formation and imbibition of colloidal inks on and in thin cellulose films — •Constantin Harder[1,2], Marie Betker[1,3], Alexakis E. Alexakis[3], Andrei Chumakov[1], Benedikt Sochor[1], Elisabeth Erbes[1,4], Marc Gensch[1,2], Qing Chen[1], Julian Heger[2], Jan Rubeck[1], Calvin Brett[1,3], Matthias Schwartzkopf[1], Eva Malmström[3], Daniel Söderberg[3], Peter Müller-Buschbaum[2], and Stephan Roth[1,3] — [1]DESY, Hamburg, Germany — [2]Lehrstuhl für Funktionelle Materialien, TUM, Garching, Germany — [3]KTH, Stockholm, Sweden — [4]Institute for X-ray Physics, Goettingen University, Goettingen, Germany

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

CPP 8.8 Wed 17:30 P

Conformation and packing of polyanions in polelyectrolyte complexes - a combined PFG and solid-state NMR study — Benjamin Kohn, Carolin Naas, Uwe Lappan, and •Ulrich Scheler — Leibniiz-Institut für Polymerforschung Dresden e.V, Dresden, Germany

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

CPP 8.9 Wed 17:30 P

Dielectric spectroscopy on lithium-salt-based deep eutectic solvents — •Arthur Schulz, Peter Lunkenheimer, and Alois Loidl — University Augsburg, Experimental Physics V

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

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

CPP 8.10 Wed 17:30 P

Poly((trifluoromethane)sulfonimide lithium styrene) as solid polymer electrolyte for lithium-ion batteries — •Fabian Alexander Christian Apfelbeck[1] and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]Heinz Maier-Leibniz Zentrum (MLZ), Technische Universität München, Garching, Germany

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

CPP 8.11 Wed 17:30 P

Influence of Mg on the structure and electrolyte/electrode interface in all-solid-state lithium battery — •Yuxin Liang and Peter Müller-Buschbaum — Technische Universität München, Fakultät für Physik, Lehrstuhl für Funktionelle Materialien, James-Franck-Str.1, 85748 Garching, Germany

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

CPP 8.12 Wed 17:30 P

Poly(propylene carbonate) as a solid polymer electrolyte — •Thien An Pham[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Technische Universität München, Physik- Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany

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

mechanical stability impeding Li dendrite growth. There has been a lot research on poly(ethylene oxide) (PEO) based SPE for the use with Li metal anodes since it offers high ionic conductivity. However, PEO is only stable up to potentials of 4V and thus, cannot be used with state of the art cathode materials like $LiNi_{1-x-y}Mn_xCo_yO_2$ that normally are operated at voltages above 4V. Aliphatic polycarbonates such as poly(ethylene carbonate) (PEC) or poly(propylene carbonate) (PPC) have intrinsically higher oxidation voltages than PEO making them suitable for high energy cathodes. Here, thin PPC films with different amount of Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt are prepared via drop casting method and studied with electrochemical impedance spectroscopy in order to determine the ionic conductivity.

CPP 8.13 Wed 17:30 P

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

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

CPP 8.14 Wed 17:30 P

Magnetic response of $CoFe_2O_4$ nanoparticles confined in PNIPAM-microgel networks — •JOACHIM LANDERS[1], MARCUS WITT[2], JURI KOPP[1], STEPHAN HINRICHS[3], SOMA SALAMON[1], BIRGIT HANKIEWICZ[3], REGINE VON KLITZING[2], and HEIKO WENDE[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Physics, TU Darmstadt — [3]Institute of Physical Chemistry, Hamburg University

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

CPP 8.15 Wed 17:30 P

2D covalent organic frameworks on monolayer MoS2 — •WENBO LU[1], DAVOR ČAČPETA[2], MIHAELA ENACHE[1], and MEIKE STÖHR[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Center of Excellence for Advanced Materials and Sensing Devices, Institute of Physics, Bijenička 46, 10000 Zagreb, Croatia

Two-dimensional (2D) transition metal dichalcogenides (TMDs) have received increasing attention as promising materials for different applications. One possibility to precisely tune the electronic and optical properties to the desired applications is based on adsorbing well-ordered organic assemblies on TMDs. Here, a study of on-surface synthesis of 2D covalent organic frameworks (COFs) on monolayer molybdenum disulfide (MoS2) on highly oriented pyrolytic graphite (HOPG) will be presented. Monolayer MoS2 films were synthesized by chemical vapor deposition and transferred to HOPG. The transferred MoS2 was characterized by atomic force microscopy and scanning tunneling microscopy (STM), from which we conclude that the transferred MoS2 is of high-quality with micrometer sized domains. For 2D COF formation, 1,4-benzenediboronic acid (BDBA) was deposited onto the MoS2/HOPG. The structure of the formed 2D COFs was studied via STM. The dehydration of BDBA results in the formation of a long-range ordered honeycomb molecular network on MoS2. Our results show the possibility of using 2D COFs to build up ordered organic/2D TMDs interfaces, which is promising for the fabrication of hybrid organic-inorganic devices possessing tailored properties.

CPP 8.16 Wed 17:30 P

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

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

CPP 8.17 Wed 17:30 P

Mesoporous ZnO thin films templated by diblock copolymer for photovoltaic applications — •TING TIAN and PETER MÜLLER-BUSCHBAUM — Physik-Department, Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-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 tailored nanostructures on the film surface are detected by surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by GISAXS.

CPP 8.18 Wed 17:30 P

Sol-gel based tailored lithium-ion battery electrodes — •IVANA PIVARNÍKOVÁ[1,2], RALPH GILLES[1], and PETER MÜLLER-BUSCHBAUM[1,2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany — [2]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

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

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

CPP 8.19 Wed 17:30 P

The influence of toluene in an Si/Ge sol-gel approach — •Christian L. Weindl[1], Christian Fajman[2], Michael A. Giebel[2], Matthias Schwarzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Lehrstuhl für Anorganische Chemie mit Schwerpunkt Neue Materialien, Chemie Department, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Notkestr.85, 22607 Hamburg, Germany — [4]Royal Institute of Technology KTH, Teknikringen 34-35, 10044 Stockholm, Sweden — [5]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 (LIBs). Owing to their high energy capacity these two group 14 semiconductors are considered as auspicious alternatives to graphite anodes in LIBs. In this study, we set the goal of synthesizing a porous silicon-germanium structure over a well-known wet chemical sol-gel approach. Here, the amphiphilic diblock copolymer polystyrene-block-polyethylene oxide (PS-b-PEO) is used as the structuring agent. In the experiment, we investigate the structural difference that occurs when toluene is used as an additive. Real-space data as SEM and EDX spectroscopy will be discussed with reciprocal-space analysis methods as GISAXS.

CPP 8.20 Wed 17:30 P

Investigation of Au(100) and Au(110) surfaces in electrolyte by Reflection Anisotropy Spectroscopy (RAS) — •Mario Löw[1], Margot Guidat[1], Timothée Gômes[1,2], Jongmin Kim[1], and Matthias M. May[1] — [1]Ulm University, Institute of Theoretical Chemistry, D-89081 Ulm — [2]Chimie Paristech - PSL, F-75005 Paris

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

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

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

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

CPP 8.21 Wed 17:30 P

Tuning the electronic and magnetic properties of graphene with periodically arranged metal-organic coordination networks — •Qiankun Wang, Brian D. Baker Cortés, Joris de la Rie, Mihaela Enache, and Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

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

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

CPP 8.22 Wed 17:30 P

bias- and concentration-dependent switching of supramolecular nanostructures at the solid-liquid interface — •Baoxin Jia[1], Mihaela Enache[1], Sandra Miguez-Lago[2], Milan Kivala[2], and Meike Stöhr[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, Netherlands — [2]Institute of Organic Chemistry, University of Heidelberg, Germany

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

CPP 8.23 Wed 17:30 P

Phase Transitions in Disordered Mesoporous Solids: Effect of Geometric Disorder — •Henry R. N. B. Enninful, Dirk Enke, and Rustem Valiullin — Leipzig University, Leipzig, Germany

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

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

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

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

CPP 8.24 Wed 17:30 P

Real-time observations of alkali metal doped 6-Phenacene films — •Matthias Zwadlo[1], Jakub Hagara[2], Giuliano Duva[1], Jan Hagenlocher[1], Alexander Gerlach[1], Martin Hodas[1], Alexander Hinderhofer[1], Peter Siffalovic[2], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Germany — [2]Institute of Physics, Slovak Academy of Sciences Bratislava, Slovakia

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

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

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

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

CPP 8.25 Wed 17:30 P

Spray-deposited anisotropic ferromagnetic hybrid polymer films of PS-b-PMMA and strontium hexaferrite magnetic nanoplatelets — •WEI CAO[1], SHANSHAN YIN[1], ANDREI CHUMAKOV[2], MATTHIAS OPEL[3], MARKUS GALLEI[4], MATTHIAS SCHWARTZKOPF[2], STEPHAN V. ROTH[2,5], and PETER MÜLLER-BUSCHBAUM[1,6] — [1]TU München, Physik-Department, 85748 Garching — [2]DESY, 22607 Hamburg — [3]WMI, Bayerische Akademie der Wissenschaften, 85748 Garching — [4]Saarland University, Chair in Polymer Chemistry, 66123 Saarbrücken — [5]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, 44 Stockholm, Sweden — [6]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) films. During spray deposition, the kinetics of structure evolution of the hybrid film is monitored in situ with grazing-incidence small-angle X-ray scattering. The obtained final hybrid film is then solvent annealed inside a closed chamber with tetrahydrofuran to study the influence of solvent vapor annealing (SVA). Due to the rearrangement of the nanoplatelets inside the DBC during SVA, an obvious change in the magnetic behavior of the hybrid film is observed. The hybrid film shows a perpendicular ferromagnetic anisotropy before SVA, which is strongly weakened after SVA. The spray deposited hybrid film appears highly promising for potential applications in magnetic data storage and sensors.

CPP 8.26 Wed 17:30 P

Influence of Chaotropic NaBr on the Swelling Behavior of PNIPMAM Thin Films — •JULIJA REITENBACH[1], CHRISTINA GEIGER[1], PEIXI WANG[1], LUCAS P. KREUZER[1], ROBERT CUBITT[2], VIET HILDEBRAND[3], ANDRÉ LASCHEWSKY[3], and PETER MÜLLER-BUSCHBAUM[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck- Str. 1, 85748 Garching — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, CS 20156, 38042 Grenoble Cedex 9, France — [3]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm

Thermoresponsive polymer thin films have gained a lot of attention in the past decades due to their attractiveness for a wide range of applications. A variety of polymer showing LCST- or UCST-type behavior are known, and their transition temperatures can be influenced by various factors such as molar mass, end groups, copolymerization or by the addition of salts. For polymers in aqueous solution, it was found that the folding of polymers can be strongly influenced by the type of salt and this ability follows a trend called the Hofmeister series. While this effect is well known in solution, the influence on the swelling behavior of PNIPMAM thin films has yet to be investigated thoroughly. We aim to elucidate the underlying mechanism by spectral reflectance and time-of-flight neutron reflectometry on a macroscopic scale and by in situ Fourier-transform infrared spectroscopy on a molecular level.

CPP 8.27 Wed 17:30 P

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

Neutron and X-Ray reflectometry are standard methods for the investigation of thin films and interfaces. Data inversion leading to a structural model is rendered difficult by the well known phase problem. Molecular Dynamics Simulations (MD) are another tool used to study interfaces. MD however has problems of its own: convergence issues and validity of the force fields, to name a few. We show here how jointly using MD and reflectometry can help elucidate details of interfacial structures such as those typically encountered in cell membranes, thin polymer films or electrochemistry. We have developed a Python software tool (Made2Reflect) which makes it easy to extract a scattering length density profile from atomistic MD and compute the corresponding reflectivity curve, thereby taking into account all aspects of the sample as well as the experimental effects such as the instrumental resolution. Actual examples will be shown illustrating that this joint method allows to (in)validate structural hypotheses which cannot be tested by means of any one of the techniques used alone.

CPP 8.28 Wed 17:30 P

Fabricating high resolution nanostructures using polymethyl methacrylate and isopropanol water mixtures — •STEPHANIE LAKE[1], FRANK HEYROTH[2], and GEORG SCHMIDT[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, MartinLuther-Universität Halle-Wittenberg, 06120 Halle, Germany

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

In this poster, we define a primary PW for polymethyl methacrylate (PMMA) during the developer stage. The area dose is varied and the range where there is sufficient development is subsequently identified. Isopropanol (IPA) and water mixtures can decrease the exposure dose needed for full development compared to other standard PMMA developers[1]. Thus, we defined yet another PW by varying the IPA concentration and measuring the aforementioned, primary PW.

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

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

CPP 8.29 Wed 17:30 P

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

Poly(2-oxazoline)s are well-known for their easy and direct synthesis, providing access to well-defined structures, with tunable properties [1]. In this study, a 1 wt% PiPOx$_{100}$-g-PEtOx$_{17}$ molecular brush with a poly(2-isopropenyl-2-oxazoline) (PiPOx) thermoresponsive backbone grafted with thermoresponsive poly(2-ethyl-2-oxazoline) (PEtOx) side chains is investigated in water-ethanol solvent mixtures. This densely grafted polymer with functional and biocompatible segments can be attractive for many applications, such as biomaterials.

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

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

CPP 8.30 Wed 17:30 P

Highly Metastable Switchable Surfaces Based on Polymer Brushes Containing End-Adsorbing Chains — •MARKUS KOCH[1], DIRK ROMEIS[1], and JENS-UWE SOMMER[1,2] — [1]Institute Theory of Polymers, IPF Dresden, Germany — [2]Institute Theory of Physics, TU Dresden, Germany

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

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

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

CPP 8.31   Wed 17:30   P

Effect of pressure on the micellar structures of PMMA-b-PNIPAM in aqueous solution — •Pablo A. Álvarez Herrera[1], Geethu P. Meledam[1], Chia-Hsin Ko[1], Bart-Jan Niebuur[1], Shu-Hsien Huang[1], Leonardo Chiappisi[2], Cristiane Henschel[3], André Laschewsky[3], Alfons Schulte[4], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]Universität Potsdam, Institut für Chemie, Potsdam-Golm, Germany — [4]University of Central Florida, Orlando, USA

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

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

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

CPP 8.32   Wed 17:30   P

Co-nonsolvency behavior of responsive polymers in thin film/vapor systems — •Christina Geiger[1], Morgan Le Dû[1], Anna Lena Oechsle[1], Peixi Wang[1], Suo Tu[1], Robert Cubitt[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionale Materialien, 85748 Garching, Germany — [2]Institut Laue-Langevin, 38000 Grenoble, France

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

CPP 9: Active Matter (joint session DY/BP/CPP)

Time: Thursday 11:45–13:00   Location: H2

CPP 9.1   Thu 11:45   H2

Orientation-dependent propulsion of active Brownian spheres: from advection to polygonal clusters* — •Jens Bickmann[1], Stephan Bröker[1], Michael E. Cates[2], and Raphael Wittkowski[1] — [1]Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Controllability of the collective dynamics of active Brownian particles is much desired for numerous potential future applications. In addition to the regular way of achieving control via external interventions, e.g., by traps, internal interventions in the dynamics of active Brownian particles become increasingly popular. Most often, internal intervention is achieved by a propulsion of the particles that depends on space, time, or orientation. Using field-theoretical modeling and particle-based simulations, we investigate systems of interacting active Brownian spheres in two spatial dimensions with an orientation-dependent propulsion. We show that different forms of orientation-dependent propulsion can give rise to advection, anomalous diffusion, and even the emergence of polygon-shaped clusters. *Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

CPP 9.2   Thu 12:00   H2

The Anomalous Transport of Tracers in Active Baths — •Omer Granek[1], Yariv Kafri[1], and Julien Tailleur[2] — [1]Department of Physics, Technion-Israel Institute of Technology, Haifa, 3200003, Israel — [2]Université de Paris, Laboratoire Matière et Systèmes Complexes (MSC), UMR 7057 CNRS, F-75205 Paris, France

We derive the exact long-time dynamics of a tracer immersed in a one-dimensional active bath. In contrast to previous studies, we find that the damping and noise correlations possess long-time tails with exponents that depend on the tracer symmetry. For an asymmetric tracer, the tails lead to superdiffusion and friction that grows with time when the tracer is dragged at a constant speed. For a symmetric tracer, we recover normal diffusion and finite friction. However, when the symmetric tracer is small compared to the active-particle persistence length, the noise becomes anticorrelated at late times and the active contribution to the friction becomes negative: active particles

then enhance motion rather than opposing it.

CPP 9.3   Thu 12:15   H2

Forces on objects immersed in active fluids — Thomas Speck and •Ashreya Jayaram — Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7-9, 55128 Mainz, Germany

Depending on their shape, objects immersed in active fluids may be subjected to a net force or net torque. We show that in a finite, periodic system, the force/torque on such an object is determined by the vorticity of the polarization of the surrounding active fluid which in turn is localized to regions close to the object where its curvature changes. We find that the system size L has a colossal influence on the magnitude of the force which grows as L^2 before saturating to a constant. We relate this force to the current away from the body and substantiate our theoretical results with numerical simulations of active Brownian particles.

CPP 9.4   Thu 12:30   H2

Active Cooling in Inertial Active Matter — •Lukas Hecht[1], Suvendu Mandal[2], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

To cool down a target domain of an equilibrium system, the system must be coupled to an external bath to which heat can be transferred. However, active matter is intrinsically out of equilibrium and the active particles themselves do not obey the second law of thermodynamics. Therefore, we ask the question if we can actively cool down active particles in a target domain without transferring a significant amount of heat to particles in the environment.

In this work, we use the active Brownian particle (ABP) model with inertia to develop a route to cool down ABPs in a target domain without the need of an external bath. Such an active cooling requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different effective temperatures [1]. Second, a mechanism that localizes the phase-separated region in the target domain is required. We show sev-

eral realizations of active cooling demonstrating how inertial effects in active matter can be utilized to actively cool down a target domain.

[1] S. Mandal, B. Liebchen, and H. Löwen, Phys. Rev. Lett. 123, 228001 (2019).

CPP 9.5   Thu 12:45   H2

Arrested phase separation in nonreciprocally interacting colloids — •Sebastian Fehlinger and Benno Liebchen — Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Non-reciprocal interactions are wide spread in nature and can lead to a huge variety of phenomenons in many physical systems. For the specific case of a binary mixture of passive particles, the breaking of the action reaction principle can lead to formation of self-propelled dimers and other active molecules. For a small system size, these active molecules have already been realized in experiments based on phoretically interacting binary colloidal mixtures [1].

This work focuses on the numerical simulation of the Langevin equations describing many noninteracting colloids which we complement with a continuum theory. We find that the nonreciprocal attractions destabilize the uniform disordered phase and lead to clusters which grow in the course of the time. Surprisingly, for a wide parameter range, the clusters only grow up to a certain size such that coarsening is arrested. We attribute this to the spatiotemporal organization of the composition of the binary mixture within the cluster which essentially screens the phoretic attractions.

[1] F. Schmidt, B. Liebchen, H. Löwen, G. Volpe, J. Chem. Phys. 150, 094905 (2019).

CPP 10: Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)

Time: Thursday 13:30–16:15   Location: H3

Invited Talk   CPP 10.1   Thu 13:30   H3

Nanophotonic structures by inkjet printing — Yidenekachew J. Donie[1], Qiaoshuang Zhang[1], Guillaume Gomard[1,2,3], and •Uli Lemmer[1,2] — [1]Light Technology Institute, Karlsruhe Institute of Technology (KIT), Germany — [2]Institute of Microstructure Technology (KIT), Karlsruhe Institute of Technology, Germany — [3]present address: Carl Zeiss AG, Eggenstein-Leopoldshafen, Germany

Inkjet printing (IJP) is a versatile method for additive manufacturing of electronic and optoelectronic devices with a typical spatial resolution on the order of 30 microns. For realizing photonic nanostructures using this approach, the deposited materials have to be controlled on a subwavelength length scale. Here, we demonstrate that this can be realized, both, in vertical and in lateral direction. Using the spontaneous phase-separation of two polymers from a common ink, we realize quasi-periodic and disordered assemblies of light scatterers. The phase separated nanostructures feature sizes that can be tuned from a few microns down to the sub-100 nm level. Applications are in the field of photonic sensors and organic optoelectronic devices. An even more precise control is necessary for realizing one-dimensional photonic crystals (dielectric mirrors) by IJP. Such an approach enables digitally controlled dielectric mirror pixels for various opto-electronic applications.

CPP 10.2   Thu 14:00   H3

On the role of interfaces in controlling the molecular orientation in thin films of polythiophenes — •Oleksandr Dolynchuk[1], Philip Schmode[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate is a superior method for inducing crystal orientation in many ordered materials. Although a preferred face-one molecular orientation was evidenced in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. By using surface-sensitive GIWAXS, here we show that thin films of P3HT crystallized on graphene exhibit a double-layered face-on and edge-on crystal orientation with the latter formed on the top surface [1]. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to graphene and vacuum. By increasing the side-chain polarity in poly[3-(6-bromohexyl)]thiophene, the influence of the interface to vacuum can be reduced, resulting in full face-on orientation in films with a thickness of up to 26 nm [1]. Our findings evidence that directed crystallization can be used to control the orientation of semicrystalline conjugated polymers in thin films if interactions with both interfaces are properly taken into account.

[1] Dolynchuk et al. Macromolecules 2021, 54, 5429-5439.

CPP 10.3   Thu 14:15   H3

Molecular Charge Transfer Effects on Perylene Diimide Acceptor and DNTT / DIP Donor Systems — •Nadine Russegger, 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 and in the excited state.

In this work, we present a comprehensive investigation on cocrystal formation and charge transfer effects in weakly interacting organic semiconductor mixtures. We choose dinaphthothienothiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different side chains in the imide position as acceptor molecules ($PDIF-CN_2$, PDIC3 and $PDIC8-CN_2$).

For a full structural overview of the resulting 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 and photoluminescence. For the various equimolar mixed systems of DNTT as well as DIP and the different perylene-diimide derivatives different charge transfer effects were determined [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the side chains and to evaluate the energy levels of the CT complexes in the different mixed systems.

[1] V. Belova et al., *J. Phys. Chem. C*, **2020**, 124, 11639-22651.

CPP 10.4   Thu 14:30   H3

Dynamics in polymer-fullerene blends for photovoltaic applications and the influence of performance enhancing measures — •Dominik M. Schwaiger[1], Wiebke Lohstroh[2], and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

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, excitons are created, subsequently dissipated at a material interface and hence free charges are provided. 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) to determine hydrogen dynamics on a pico- to nanosecond timescale. In addition, two well established techniques for performance enhancement in organic photovoltaics, namely the addition of DIO to the casting solution and a methanol posttreatment of the active layer, are applied and their influence on the polymer dynamics is investigated.

CPP 10.5   Thu 14:45   H3

Thermally Evaporated Donor Molecules Well-Suited for Low-Voltage Loss Organic Solar Cells — •Pascal Kaienburg[1], Helen Bristow[2], Anna Jungbluth[1], Irfan Habib[1], David Beljonne[3], and Moritz Riede[1] — [1]Clarendon Laboratory, Department of Physics, University of Oxford, UK — [2]Department of Chem-

istry, University of Oxford, UK — [3]Laboratory for Chemistry of Novel Materials, University of Mons, Belgium

Novel molecules are key drivers in the development of efficient organic solar cells (OSCs). Device fabrication via solution-casting, mostly of polymer-blends, and thermal evaporation of small molecule blends in vacuum have proven successful. The advent of non-fullerene acceptors (NFAs) in solution processing pushed OSC efficiency by 50%, outpacing the development of vacuum-deposited OSCs.

We take an important first step towards efficient NFA-based evaporated OSCs by demonstrating that donors commonly used in vacuum deposition benefit from being combined with NFAs. We do so by evaporating donors onto solution-cast NFAs and performing in-depth analysis of voltage losses via sensitive EQE and electroluminescence on the resulting bilayer devices. We find that voltage losses of donor/NFA systems are reduced by up to 400mV compared to corresponding donor/C60 systems, without compromising photocurrent.

Together with evaporated OSCs' advantages such as industrial scalability as proven by OLEDs, our findings highlight the technology's potential and stress the need for evaporable non-fullerene acceptors, which - once available - will significantly increase OSC efficiency.

15 min. break

CPP 10.6   Thu 15:15   H3

Cellulose-silver nanoparticle composites for optical applications — Calvin J. Brett[1,2], Björn Fricke[1], Alexandros E. Alexakis[2], Tim Laarmann[1,3], Volker Körstgens[4], Peter Müller-Buschbaum[4,5], Daniel Söderberg[2], and •Stephan V. Roth[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — [3]The Hamburg Centre for Ultrafast Imaging CUI, 22761 Hamburg, Germany — [4]Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität Muenchen, 85748 Garching, Germany — [5]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität Muenchen, 85748 Garching, Germany

Cellulose nanofibrils (CNF) provide biocompatibility and are emerging candidates for functional composites and for templating organic optoelectronics. Here we present a facile fabrication of biocompatible hybrid thin films with tunable optical responses by establishing a thin film composite of silver nitrate precursor and CNF films. Subsequent thermal annealing induces the transformation of the silver nitrate into metallic silver nanoparticles and their CNF-template assisted growth. Correlating nanoparticle morphology and optical spectroscopy, our results show the ability to tailor the electronic band gap of the silver nanoparticles and thus of the hybrid material by adjusting the time scale of the thermal transformation.

[1] Brett et al., ACS Appl. Mater. Interfaces 13, 27696 (2021)

CPP 10.7   Thu 15:30   H3

Tunability of the Circular Dichroism through Photoluminescent Moiré Patterns — •Olha Aftenieva[1] and Tobias A.F. König[1,2] — [1]Leibniz Institute for Polymer Research Dresden e.V. Hohe Straße 6, 01069 Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed) Technische Universität Dresden 01062 Dresden, Germany

In nanophotonics, there is a current demand for ultrathin, flexible nanostructures that are simultaneously easily tunable, demonstrate a high contrast, and have a strong response in photoluminescent polarization. In this work, the template-assisted self-assembly of water-dispersed colloidal core-shell quantum dots into 1D light-emitting submicrometer gratings on a flexible substrate is demonstrated. Combining such structures with a light-absorbing metallic counterpart by simple stacking at various angles results in a tunable Moiré pattern with strong lateral contrast. Furthermore, a combination with an identical emitter-based grating leads to a chiroptical effect with a remarkably high degree of polarization of 0.72. Such a structure demonstrates direct circular polarized photoluminescence, for the first time, without a need for an additional chiral template as an intermediary. The suggested approach allows for reproducible, large-area manufacturing at reasonable costs and is of potential use for chiroptical sensors, photonic circuit applications, or preventing counterfeit.

CPP 10.8   Thu 15:45   H3

Ultrafast Energy Conversion in Organic Photovoltaic Materials: First-principles modelling of the prototypical P3HT-PCBM blend heterojunction — •Elisa Palacino-González and Thomas la Cour Jansen — University of Groningen, Faculty of Science and Engineering, Nijenborgh 4, 9747 AG Groningen

One of the reasons behind the low energy conversion efficiency of organic photovoltaic cells has been ascribed to electronic-vibrational dynamics affecting the ultrafast charge separation material upon light absorption. The absence of a comprehensive theoretical description of this process has restrained further advancements in this direction. Here the first step towards this is presented by introducing a first-principles modelling of the key prototype P3HT-PCBM heterojunction system with a realistic description of the blend environment. MD simulations with the GROMOS 53A6 force field are performed to determine structural and dynamical properties of the blend. Representative strongly coupled subsystems of donor-acceptor pairs with a few P3HT-PCBM moieties are selected from the MD structures, with the bright donor state localised on the P3HT molecule and the charge transfer state with a hole on P3HT and the electron on PCBM. Using an electronic basis, the Hamiltonian includes localised excitons and charge transfer states. Excitation energies fluctuating along the MD trajectory are determined using TDDFT and an electrostatic mapping scheme, which are used to define the spectral densities of the system-bath coupling. The resultant molecular Hamiltonian will be used in the quantum dynamical and spectral simulations in the following step.

CPP 10.9   Thu 16:00   H3

Understanding directional charge transfer in a bacterial reaction center: effect of molecular vibrations — •Mario Marques[1] and Linn Leppert[2,1] — [1]Institute of Physics, University of Bayreuth, Bayreuth 95440, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The primary energy conversion reactions of photosynthesis in purple bacteria occur in the reaction center (RC), a complex structure in which photo-active pigments arranged along two pseudo-symmetric branches mediate excitation and charge transfer. Our previous first-principles calculations of optical excitations in the RC of *Rhodobacter sphaeroides* indicated that charge transfer occurs along both pigment branches, in contradiction with well-established experimental observations that show charge transfer along only one branch. In this work, we use (time-dependent) density functional theory to investigate the influence of molecular vibrations on the excited states of the main RC pigments of purple bacteria, to unravel their role in the directional charge transfer.

CPP 11: Thin Oxides and Organic Thin Films (joint session DS/CPP)

Time: Thursday 15:15–16:15 Location: H5

CPP 11.1 Thu 15:15 H5

Hybrid electronic states in epitaxially layered perovskite oxide electrocatalysts for water electrolysis — •Lisa Heymann[1], Moritz Weber[1], Marcus Wohlgemuth[1], Felix Gunkel[1], and Christoph Baeumer[1,2] — [1]Peter Gruenberg Institute and JARA-FIT, Forschungszentrum Juelich GmbH, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

In electrochemical water splitting catalyzed by perovskite oxides (ABO_3), the B-O hybridization degree has a major impact on the electrocatalytic activity. Additionally, space charge layers at the interface to the electrolyte may hamper the electron transfer into the electrode, complicating the analysis of hybridization phenomena. The goal in this work was to explore whether A site doping in cobaltites ($ACoO_3$) has a major impact on the oxygen evolution reaction (OER) through a different degree of hybridization or the extend of a surface space charge layer. We investigated $La_{0.6}Sr_{0.4}CoO_3$ and $LaCoO_3$ bilayer structures in epitaxial thin films that enabled us to create a near surface depth profile of both, the hybridization degree and the doping concentration confirmed by x-ray photoelectron spectroscopy (XPS). In a Mott Schottky (MS) analysis, we showed that in the OER potential regime the catalytic activity is not limited by a space charge layer. Therefore, we can correlate the observed OER activity trend to the degree of hybridization in cobaltites. The combined XPS and MS analysis enables to differentiate between the influence of the hybridization degree and intrinsic space charge layers, which are indistinguishable in a sole physical or electrochemical characterization.

CPP 11.2 Thu 15:30 H5

tailored electrical characteristics in TiOx/HfOx-based memristive device for targeting neuromorphic computing — •Seongae Park[1,2], Stefan Klett[1], Tzvetan Ivanov[1,2], Andrea Knauer[2], Joachim Doell[2], and Martin Ziegler[1,2] — [1]Department of Electrical Engineering and Information Technology, TU Ilmenau, Ilmenau, Germany — [2]Institute of Micro and Nanotechnologies MacroNano, TU Ilmenau, Ilmenau, Germany

Over the last few years, memristive devices have shown their high potential for neuromorphic computing. In particular, redox-based memristive devices have become the focus of research interest, since they enable precise emulation of synaptic functionality through local ionic processes. However, for targeted device functionality, a detailed understanding of ionic processes at the atomic level is required, which is often severely hampered by coupled electronic and ionic processes. In this talk, the bi-layer oxide system TiOx/HfOx is presented. In a combined approach using a 4-inch wafer process technology and a physical device model, we show the contribution of physical device parameters such as device area size, the thickness of HfOx, interface modification, as well as the stoichiometry of HfOx to the electrical characteristics. Furthermore, we present how those parameters can be tuned for customized device functionalities. In that respect, memristive devices with tailored I-V characteristics and analog resistive switching are obtained that own an intrinsic self-compliance and do not need electroforming-free cycles.

CPP 11.3 Thu 15:45 H5

Arrangement and electronic properties of cobalt phthalocyanine molecules on Si(111) $(\sqrt{3} \times \sqrt{3})$ R30°-B — •Milan Kubicki, Martin Franz, Susi Lindner, Holger Eisele, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The formation of self-assembled monolayers of organic molecular materials on solid surfaces is an important subject because of their possible application in advanced optical and electronic devices. Here, the molecular arrangement and the interfacial electronic properties of cobalt phthalocyanine (CoPc) on the deactivated Si(111) $(\sqrt{3} \times \sqrt{3})$ R30°-B surface are studied by scanning tunneling microscopy and spectroscopy [1,2]. It is found that for submonolayer coverages the CoPc molecules lie flat on the Si surface with the Co d_{z^2} orbital of the molecule forming a hybrid state with the p_z orbital of the Si adatom at the surface. For multilayer coverages in contrast, the CoPc molecules are tilted with respect to the Si surface forming highly ordered organic molecular films, and the electronic properties resemble those of pure CoPc.

[1] S. Lindner, M. Franz, M. Kubicki, S. Appelfeller, M. Dähne, and H. Eisele, Phys. Rev. B **100**, 245301 (2019).
[2] M. Kubicki, S. Lindner, M. Franz, H. Eisele, and M.Dähne, J. Vac. Sci. Technol. B **38**, 042803 (2020).

CPP 11.4 Thu 16:00 H5

Experimental Quantification of Interaction Energies in Organic Monolayers — •Pierre-Martin Dombrowski, Stefan Renato Kachel, Leonard Neuhaus, Tobias Breuer, J. Michael Gottfried, and Gregor Witte — Philipps-Universität Marburg, Germany

The formation of molecular nanostructures is determined by the interplay of intermolecular and molecule-substrate interactions. However, these interactions are experimentally hardly accessible. Temperature-programmed desorption (TPD) is a fairly well-established experimental technique capable of quantifying both types of interaction, but its quantitative analysis is by no means trivial. In the present study, we analyse the desorption kinetics of the two organic semiconductors pentacene (PEN) and perfluoropentacene (PFP) from Au(111) and MoS_2 surfaces to show the potential of TPD, but also highlight challenges for large adsorbates. Combining TPD with scanning tunnelling microscopy, work function measurements and theoretical modelling, we show that intermolecular interactions are dominated by the intramolecular charge distribution, resulting in net intermolecular repulsion in unitary and attractive interactions in mixed PEN:PFP monolayers. We determine the coverage-dependent prefactor of desorption with unprecedented precision and correlate its evolution with the activation of specific degrees of freedom of motion of adsorbed molecules. Lastly, we compare differences in molecule-substrate interactions on Au(111) and MoS_2, revealing that (sub-)monolayers on MoS_2 are stabilized only by entropy.

CPP 12: Annual General Meeting of the CPP Division (CPP Mitgliederversammlung)

Virtual Zoom Meeting - Report of the current speaker team - Election of the second deputy speaker - Miscellaneous

(Link will be available via the CPP newsletter)

Time: Thursday 17:30–18:30 Location: MVCPP
Virtual Zoom Meeting

CPP 13: Molecular Electronics, Hybrid and Perovskite Photovoltaics

Time: Friday 10:00–12:45   Location: H3

Invited Talk   CPP 13.1   Fri 10:00   H3
Electron-lattice relaxation effects in halide perovskites —
•David A. Egger — Technichal University of Munich, Germany

Halide perovskites (HaPs) have shown great promise as materials for applications in energy and optoelectronic devices owing to their fascinating microscopic properties. Of particular scientific interest is the coupling of electronic to lattice-dynamical properties of HaPs, because a comprehensive understanding of it is key to predicting and further improving charge-carrier and optical transport characteristics. In this talk, I will present our recent theoretical findings on electron-lattice relaxation effects in HaPs. Specifically, using molecular dynamics in conjunction with electronic-structure theory, it will be shown that the soft, polar lattice of paradigmatic HaPs leads to a variety of very interesting electron-lattice relaxation phenomena. These include structural anharmonicities, nonlinear electron-phonon couplings and short-range correlated disorder potentials. It will be demonstrated that these mechanisms are key to a microscopic picture of charge-carrier mobilities and optical absorption properties of HaPs.

CPP 13.2   Fri 10:30   H3
In situ GIXS study on the crystallization and mesoscale film formation of lead-free MBI perovskite on mesoporous titania during spray deposition from a green solvent — •Julian E. Heger[1], Marie Betker[2,3], Constantin Harder[1,3], Benedikt Sochor[3], Christian L. Weindl[1], Matthias Schwartzkopf[3], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany — [2]Royal Institute of Technology KTH, Teknikringen 34-35, 100 44 Stockholm, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Hybrid halide perovskites are highly promising materials in photovoltaics, due to high efficiencies and industrial favorable processability. However, most of the studied systems are based on water-soluble lead and toxic solvents, which lower the broad application within European standards of hazardous materials. Bismuth-based alternatives like methylammonium bismuth iodide (MBI) can offer a green route to lead-free perovskite solar cells on a large scale when synthesized in the comparably non-toxic solvent methyl acetate and processed by industrially applicable spray deposition. In this work, we investigate with in situ synchrotron GIXS the crystallization and mesoscale film formation of MBI perovskite on mesoporous titania during spray deposition, to understand MBI formation on a typical solar cell interface.

CPP 13.3   Fri 10:45   H3
In situ GIWAXS phase and texture tracking of 2-step slot-die coated perovskite — •Manuel Andree Scheel[1], Lennart Klaus Reb[1], Renjun Guo[1], Matthias Schwartzkopf[2], Stephan Volkher Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]DESY, 22607 Hamburg, Germany — [3]KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — [4]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Perovskite slot-die coating is a promising thin-film deposition technique for organic-inorganic perovskite materials and might lead the way towards commercial high efficient solar cells. Roll-to-roll compatible deposition techniques offer the possibility to combine high production throughput with minimal waste, and offer high customizability at the same time. 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). Here, we study the thin-film morphology and texture of the resulting thin film during the annealing process. We track the phase evolution and their respective crystal orientations over time. We find, that the precursor-solvent phase influences the final crystal orientation in the thin-film by acting as a precursor source that controls the level of available precursor material. We also investigate deposition-technique depending differences that can influence thin-film characteristics.

15 min. break

CPP 13.4   Fri 11:15   H3
Perovskite and Organic Solar Cells Generate Power in Space — •Lennart Klaus Reb[1], Michael Böhmer[1], Benjamin Predeschly[1], Sebastian Grott[1], Christian Ludwig Weindl[1], Goran Ivkovic Ivandekic[1], Renjun Guo[1], Christoph Dreissigacker[2], Jörg Drescher[2], Roman Gernhäuser[1], Andreas Meyer[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Garching, DE — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, DE — [3]Heinz Maier-Leibnitz-Zentrum, Garching, DE

Perovskite and organic solar cells have become a hot research topic in the last few years. The lightweight thin-film solar cells are of particular interest for space applications due to their exceptional power per mass, exceeding their inorganic counterparts by magnitudes.

Here, we present the Organic and Hybrid Solar Cells In Space experiment (OHSCIS) and the launch of perovskite and organic solar cells to space for the first time [1, 2]. The mechanical and electronic design of the experiment aims at maximizing the data collection rate and precise measurements. We show that the solar cells operate in space conditions and produce reasonable power per area of up to 14 and 7 mW cm-2, respectively. Also, during a phase being turned away from the Sun, the solar cells produce power from collecting faint Sun-light scattered from Earth. Our results highlight the potential for near-Earth applications and 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
[2] L. Reb et al., Rev. Sci. Instrum. 92 (2021), doi.org/10.1063/5.0047346.

CPP 13.5   Fri 11:30   H3
Optimally-tuned range-separated hybrid functionals for accurate molecular excited-state geometries — •Bernhard Kretz and David A. Egger — Technical University of Munich, Germany

Molecular excited-state (ES) potential energy surfaces (PES) obtained by computational methods can shed light on reaction mechanisms and pathways in photocatalytic reactions. These ES PES can be calculated using either time-dependent density functional theory (TD-DFT) or high-level wave-function methods. TD-DFT based calculations are computationally very efficient, but often lack the accuracy achieved by computationally more expensive wave-function methods[1]. Recently, the class of optimally-tuned range-separated hybrid (OT-RSH) functionals[2] was developed which promises to reduce the gap in accuracy.

In our recent work[3], by comparison with high accuracy wave-function data from literature, we assessed the accuracy of TD-DFT and OT-RSH for the excited-state geometries for a selection of organic molecules with varying complexity of their ES PES. We mainly focused on the structural parameters of the lowest-excited singlet states. Our results show that OT-RSH maintains the accuracy of conventional functionals for small molecules, while it improves the description of more complex ES PESs involving charge-transfer states.

[1] C. Azarias, J. Phys. Chem. A, 121, 32, 6122 (2017)
[2] L. Kronik et al., J. Chem. Theory Comput., 8, 5, 1515 (2012)
[3] B. Kretz and D. A. Egger, J. Chem. Theory Comput., 17, 1, 357 (2021)

Invited Talk   CPP 13.6   Fri 11:45   H3
Light-actuated colloidal nano- and microparticles —
•Cornelia Denz[1], Matthias Rueschenbaum[1], Valeria Bobkova[1], Julian Jeggle[2], and Raphael Wittkowski[2] — [1]Institute of Applied Physics, University of Muenster — [2]Institute of Theoretical Physics, University of Muenster

Propelled colloidal particles constitute biomimetic analogues to natural microswimmers and represent ideal agents for responsive and adaptive soft matter. Among the numerous propulsion mechanisms developed recently to self-propel such nano- and microparticles, light is a most promising stimulus, since it enables a natural spatio-temporal control of the motion, especially for large numbers of the particles, leading to swarming-like behaviour or novel active materials with exceptional properties.

We introduce on the one hand a novel class of such particles that are light-actuated based on symmetry-broken refraction, fabricated by

3d laser printing based on two-photon polymerization. By numerical simulations, we will discuss collective, light-actuated effects including unexpected patterns and transport effects.

On the other hand, we demonstrate that light actuation of a large number of colloidal particles in optical feedback leads to self-organized pattern formation including the superposition of symmetric patterns as hexagons, rolls and squares. We discuss the stability of these patterns and their control.

CPP 13.7 Fri 12:15 H3
Laser-Induced Electronic and Vibronic Dynamics in the Pyrene Molecule and its Cation — •KATHERINE R. HERPERGER[1,2], JANNIS KRUMLAND[2], and CATERINA COCCHI[2,3] — [1]Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada — [2]Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany — [3]Carl von Ossietzky Universität Oldenburg, Institute of Physics, 26129 Oldenburg, Germany

Among polycyclic aromatic hydrocarbons (PAHs), pyrene ($C_{16}H_{10}$) is widely used as an optical probe thanks to its unique ultraviolet absorption and infrared emission features. In this first-principles study based on real-time time-dependent density-functional theory coupled with the Ehrenfest molecular dynamics scheme, we investigate the subpicosecond electronic and vibronic response of a pyrene molecule and its cation excited by a coherent ultraviolet Gaussian pulse. The response of both the species is analyzed in terms of electronic population, absorption spectra, and vibrational activity. Combining this knowledge with the symmetry properties of pyrene, we gain insight into the transient response of this molecule to laser perturbation, setting the stage for future studies on larger and more complex PAHs.

CPP 13.8 Fri 12:30 H3
Charge transfer dynamics across the Au/Ferrocene (aq) interface studied by a two photon pump - photovoltage probe scheme — •MANUEL BRIDGER, ZHIPENG HUANG, YUJIN TONG, OSCAR NARANJO, ALEXANDER TARASEVITCH, RICHARD KRAMER CAMPEN, and UWE BOVENSIEPEN — University Duisburg/Essen

Photo-excitation at interfaces redistributes electrons between bulk phases on microscopic spatial and ultrafast time scales. Here we employ a two photon pump - photovoltage probe scheme to quantify the relationship of particular resonant optical transitions to interfacial charge redistribution for the case of charge transfer between a gold electrode and ferrocene self assembled monolayer in an electrochemical cell. We access vibrational and electronic excited states of ferrocene with femtosecond pulses of center wavelength 3 μm and 400 nm respectively. Two signals are apparent: a large amplitude voltage transient at 120 ± 80 fs and a small at 4.0 ± 2.7 ps. Control experiments and comparison to similar systems probed in vacuum by 2PPE spectroscopy suggest the former is the result of charge transfer via vibronically coupled ferrocene CH vibration and hybrid ferrocene/Au electronic states and the later charge transfer via vibrationally mediated interfacial polarization. These results imply that stabilising such vibronically coupled states is a useful target for devices that rely on efficient charge transfer at solid/liquid interfaces.

CPP 14: Condensed-Matter Simulations augmented by Advanced Statistical Methodologies (joint session DY/CPP)

Time: Friday 10:00–11:00 Location: H2

CPP 14.1 Fri 10:00 H2
Simple model to describe stability of thin domains — •RUBEN KHACHATURYAN[1], ARNE J. KLOMP[2], KARSTEN ALBE[2], and ANNA ANNA GRÜNEBOHM[1] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-University Bochum — [2]Department of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

Ferro domains are important for contemporary electronics, particularly decreasing domain size allowing for denser information storage per unit area. Thermal fluctuations limit domain stability, which is the key property for ferroic data storage. Therefore the ability to estimate the expected lifetime of a domain is of crucial importance. In this work, we simulate 180° domains in BaTiO3 with different widths at various temperatures using ab initio based molecular dynamics simulation employing LAMMPS and feram codes. We then derived a model to analyze the lifetime of the domains depending on their width and temperature. The model treats domain walls as fluctuating strings. String stiffness reflects the information about energy for domain wall roughening and thermal fluctuations are considered as a field of random forces. Our findings allowed us to interpret the stochastic nature of thin domain collapses and identify associated energies. With further development of the model, we are planning to consider the behavior of ferroelastic and ferromagnetic domain walls.

CPP 14.2 Fri 10:15 H2
Population Annealing Monte Carlo Using the Rejection-Free n-Fold Way Update Applied to a Frustrated Ising Model on the Honeycomb Lattice — •DENIS GESSERT[1,2] and MARTIN WEIGEL[1,3] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Population annealing (PA) is a MC method well suited for the study of systems with a rough free energy landscape, e.g. glassy systems. PA is similar to an equilibrium version of parallel simulated annealing runs with the addition of a resampling step at each temperature. While a large population may improve imperfect equilibration, it is evident PA will fail when almost no spins are flipped in the equilibration routine.

This is the case in systems with a low temperature phase transition where high Metropolis rejection rates make sampling phase space near infeasible. To overcome this slowdown we propose a combination of the PA framework with the rejection-free "n-fold way" update and achieve an exponential speed-up at low temperatures compared to Metropolis.

To test our method we study the Ising model with competing ferromagnetic nearest and antiferromagnetic next-to-nearest neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, resp., on the honeycomb lattice. As T_c becomes arbitrarily small, when approaching the special point $J_2 = -J_1/4$ with $T_c = 0$, we consider this a good choice to test the efficacy of our method.

CPP 14.3 Fri 10:30 H2
Noncontact friction: The role of viscous friction and its non-universality — •MIRU LEE[1], NIKLAS WEBER[2], RICHARD VINK[2], CYNTHIA VOLKERT[2], and MATTHIAS KRÜGER[1] — [1]Institut für Theoretische Physik, Friedrich- Hund-Platz 1, 37077 Göttingen — [2]Institut für Materialphysik, Friedrich-Hund-Platz 1, 37077 Göttingen

Obtaining theoretical predictions for friction during sliding motion is challenging due to the complex nature of the problem. In the so-called noncontact regime, the friction tensor is given by the leading order of the pairwise interactions between the probe and the surface atoms [1]. In such a regime, one can thus find an analytic expression of the friction tensor [2]. Starting from a stochastic viscoelastic solid model, we identify the two paradigmatic dissipation mechanisms [3]: phonon radiation, prevailing even in a purely elastic solid, and phonon damping, e.g., caused by viscous motion of crystal atoms. At small probe-surface separations, phonon damping dominates over phonon radiation, and vice versa at large separations. Phonon radiation is furthermore universal; there exists a general one-to-one mapping between the mean probe-surface force and the resulting friction. In contrast, phonon damping is non-universal, and no such general relation exists; it is subject to the details of the underlying pairwise interaction, e.g., the interaction range. For certain cases, the friction can even *decrease* with increasing surface area the probe interacts with.
[1] M. Lee, R. Vink, M. Krüger, Phys. Rev. B **101**, 235426 (2020)
[2] A. I. Volokitin, et. al., Phys. Rev. B **73**, 165423 (2006)
[3] M. Lee, R. Vink, C. Volkert, M. Krüger, In preparation.

CPP 14.4 Fri 10:45 H2
Investigation of transferability in LDOS based DFT surrogate models for multiscale simulations — •LENZ FIEDLER[1,2] and ATTILA CANGI[1,2] — [1]Center for Advanced Systems Understanding (CASUS) — [2]Helmholtz-Zentrum Dresden-Rossendorf

Density Functional Theory (DFT) is one of the most important computational tools for materials science, as it combines high accuracy with general computational feasibility. However, applications important to scientific progress can pose problems to even the most advanced and efficient DFT codes due to size and/or complexity of the underlying simulations. Namely the modeling of materials across multiple length and time scales at ambient or extreme conditions, necessary for the understanding of important physical phenomena such as radiation damages in fusion reactor walls, evade traditional ab-initio treatment. DFT surrogate models are a useful tool in achieving this goal by reproducing DFT results at drastically reduced computational cost by using machine learning methods. Yet, a lack of transferability of many approaches lead to repeated and costly training data generation procedures. Here, we present results of an investigation to transfer such machine learning DFT surrogate models between different simulation cell sizes, with the goal of reducing the overall amount of computational time for training data generation. The models are based upon the Materials Learning Algorithms (MALA) package [1] and the therein implemented LDOS based machine learning workflow [2].

[1]: https://github.com/mala-project
[2]: J. A. Ellis et al., Phys. Rev. B 104, 035120, 2021

CPP 15: Theory and Simulation (joint session CPP/DY)

Time: Friday 13:30–15:00   Location: H3

Invited Talk   CPP 15.1   Fri 13:30   H3
Data-driven protein design and simulation — •Andrew Ferguson — University of Chicago, Chicago, IL, USA

Data-driven modeling and deep learning present powerful tools that are opening up new paradigms and opportunities in the understanding, discovery, and design of soft and biological materials. In this talk, I will first describe an approach integrating ideas from dynamical systems theory, nonlinear manifold learning, and deep learning to reconstruct protein folding funnels and molecular structures from one-dimensional time series in experimentally measurable observables obtainable by single molecule FRET. I will then describe our recent development and application of deep representational learning to expose the sequence-function relationship within homologous protein families and to use these principles for data-driven design of synthetic proteins with new and/or elevated function.

CPP 15.2   Fri 14:00   H3
Are there knots in chromatin? — •Peter Virnau — Institut für Physik, Staudingerweg 9, Johannes Gutenberg-Universität Mainz, 55128 Mainz

The rise of HiC chromosome capture methods has recently enabled low-resolution structures of interphase chromatin [1]. In this presentation I will explain how structures based on single cell contact matrices are obtained from simulations of coarse-grained bead-spring polymer Go models [2]. The role of self-entanglements which naturally occur in this process [2,3] will be critically assessed in the light of theoretical arguments and recent experiments [4].

[1] T.J. Stevens et al, Nature 544, 59-64 (2017). [2] S. Wettermann et al, Comp. Mat. Sci 173, 109178 (2020). [3] J.T. Siebert et al, Polymers 9, 317 (2017). [4] D. Goundaroulis, Biophys. J. 118, 2268-2279 (2020).

CPP 15.3   Fri 14:15   H3
Surface Segregation in Athermal Polymer Blends due to Conformational Asymmetry — •Russell Spencer[1] and Mark Matsen[2] — [1]Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany — [2]University of Waterloo, Waterloo, Ontario, Canada

Monte Carlo simulations are used to investigate the surfaces of athermal blends of stiff and flexible polymers. We vary the bending modulus of the stiff polymers, κ, from zero to the point where the bulk undergoes an isotropic-to-nematic transition. For hard walls characteristic of polymer/solid surfaces, the flexible polymers generally segregate to the surface. However, prior to the bulk transition, there is a surface ordering transition, where a thin nematic layer rich in stiff polymers forms at the surface. On increasing κ further, the thickness of the nematic layer rapidly increases as the bulk isotropic-to-nematic transition is approached. For soft boundaries representative of polymer/air surfaces, a thin layer rich in stiff polymers but without nematic order forms on the outer edge of the surface with a more significant layer rich in the flexible chains beneath. In this case, the nematic layer never appears, and the surface profile evolves continuously with increasing κ.

CPP 15.4   Fri 14:30   H3
Ultra-coarse-graining of homopolymers in inhomogeneous systems — •Fabian Berressem[1], Christoph Scherer[2], Denis Andrienko[2], and Arash Nikoubashman[1] — [1]Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Polymer Research, Mainz

We develop coarse-grained (CG) models for simulating homopolymers in inhomogeneous systems, focusing on polymer films and droplets. If the CG polymers interact solely through two-body potentials, then the films and droplets either dissolve or collapse into small aggregates, depending on whether the effective polymer-polymer interactions have been determined from reference simulations in the bulk or at infinite dilution. To address this shortcoming, we include higher order interactions either through an additional three-body potential or a local density-dependent potential (LDP). We parameterize the two- and three-body potentials via force matching, and the LDP through relative entropy minimization. While the CG models with three-body interactions fail at reproducing stable polymer films and droplets, CG simulations with an LDP are able to do so. Minor quantitative differences between the reference and the CG simulations, namely a slight broadening of interfaces accompanied by a smaller surface tension in the CG simulations, can be attributed to the deformation of polymers near the interfaces, which cannot be resolved in the CG representation, where the polymers are mapped to spherical beads.

CPP 15.5   Fri 14:45   H3
How to accurately estimate the specific heat of liquid polymers? — •Debashish Mukherji[1], Hongyu Gao[2], Tobias P. W. Menzel[2], and Martin H. Mueser[2] — [1]Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [2]Department of Materials Science and Engineering, Saarland University, 66123 Saarbruecken, Germany

The field of atomistic simulations of polymers is in a mature stage, yet predictions of specific heat from molecular simulations and successful comparisons with experimental data are scarce if existing at all. One reason for this may be that the internal energy and thus the specific heat cannot be coarse-grained so that they defy their rigorous computation with united-atom models. Moreover, many modes in a polymer barely contribute to the specific heat because of their quantum mechanical nature. Here, we adopt an existing method [1], which defines a specific heat for a harmonic reference, to estimate the specific heat difference between classical and quantum-mechanical systems and use this as a correction factor. Thereby, we predominantly correct the stiff, high-frequency harmonic modes, while leaving the specific-heat contributions of the slow (anharmonic) modes intact [2]. We show how to construct corrections for both all-atom and united-atom descriptions of chain molecules. Corrections computed for a set of hydrocarbon oligomers and commodity polymers deviate by less than kB/10 per particle. The results compare well with experimental data.

[1] Horbach, Kob, and Binder, JPCB 103, 4104 (1999). [2] Gao, Menzel, Mueser, and Mukherji, PRM 5, 065605 (2021).