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Overview of Invited Talks and Sessions

(Lecture halls H38 and H39; Poster P1 and P2)

Invited Talks

CPP 1.1	Mon	9:30–10:00	H38	**Ternary blend approach for boosting performance and stability of organic solar cells** — •Tayebeh Ameri
CPP 8.1	Mon	15:00–15:30	H38	**Stimuli-Responsive Opal Films based on Core-Shell Particle Self-Assembly** — •Markus Gallei
CPP 8.3	Mon	15:45–16:15	H38	**Self-assembled photonic pigments from bottlebrush block copolymers** — •Richard Parker, Tianheng Zhao, Zhen Wang, Clement Chan, Silvia Vignolini
CPP 8.5	Mon	16:45–17:15	H38	**Hierarchically structured mechanochromic deformation-sensing pigments** — •Jessica Clough, Cédric Kilchoer, Bodo Wilts, Chris Weder
CPP 13.1	Tue	9:30–10:00	H38	**Insights into degradation mechanisms in Li-based batteries and advantages of polymer coatings** — •Neelima Paul
CPP 18.1	Tue	11:30–12:00	H38	**How X-rays can reveal waters mysteries** — •Katrin Amann-Winkel
CPP 19.1	Wed	9:30–10:00	H38	**Elucidating the role of antisolvent polarity on the surface chemistry and optoelectronic properties of lead-halide perovskite nanocrystals** — •Robert Hoye
CPP 33.1	Thu	9:30–10:00	H38	**Cooperative and non-Gaussian dynamics of entanglement strands in polymer melts** — •Margarita Kruteva, Michaela Zamponi, Ingo Hoffmann, Jürgen Allgaier, Lutz Willner, Andreas Wischnewski, Michael Monkenbusch, Dieter Richter
CPP 37.1	Thu	10:30–11:00	H39	**Non-equilibrium Properties of Thin Polymer Films** — •Günter Reiter, Sivasurender Chandran
CPP 40.1	Thu	15:00–15:30	H38	**Computational Design of Organic Semiconductors** — •Harald Oberhofer
CPP 41.1	Thu	15:00–15:30	H39	**Interface-induced crystallization in polymers: From model systems to applications for semiconducting polymers** — Muhammad Tariq, Robert Kahl, Mukundan Thelakkat, Thomas Thurn-Albrecht, •Oleksandr Dolynchuk
CPP 44.1	Fri	9:30–10:00	H38	**Connecting dynamics and phase behavior of proteins: The neutron perspective** — •Frank Schreiber
CPP 44.5	Fri	10:45–11:15	H38	**Magnetic particle self-assembly at functionalized interfaces** — •Max Wolff
CPP 45.1	Fri	9:30–10:00	H39	**New biobased material concepts using scattering techniques to elucidate and control nanoscale assembly** — •Daniel Söderberg

Invited Talks of the joint Symposium SKM Dissertation Prize 2022 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	10:15–10:45	H2	**Charge localisation in halide perovskites from bulk to nano for efficient optoelectronic applications** — •Sascha Feldmann
SYSD 1.2	Mon	10:45–11:15	H2	**Nonequilibrium Transport and Dynamics in Conventional and Topological Superconducting Junctions** — •Raffael L. Klees
SYSD 1.3	Mon	11:15–11:45	H2	**Probing magnetostatic and magnetotransport properties of the antiferromagnetic iron oxide hematite** — •Andrew Ross
SYSD 1.4	Mon	11:45–12:15	H2	**Quantum dot optomechanics with surface acoustic waves** — •Matthias Weiss

Invited Talks of the joint Symposium From Physics and Big Data to the Design of Novel Materials (SYNM)

See SYNM for the full program of the symposium.

SYNM 1.1	Mon	15:00–15:30	H1	**How to tackle the "I" in FAIR?** — •Claudia Draxl
SYNM 1.2	Mon	15:30–16:00	H1	**Beyond the average error: machine learning for the discovery of novel materials** — •Mario Boley, Simon Teshuva, Felix Luong, Lucas Foppa, Matthias Scheffler
SYNM 1.3	Mon	16:00–16:30	H1	**The Phase Diagram of All Inorganic Materials** — •Chris Wolverton
SYNM 1.4	Mon	16:45–17:15	H1	**Automated data-driven upscaling of transport properties in materials** — •Danny Perez, Thomas Swinburne
SYNM 1.5	Mon	17:15–17:45	H1	**Data-driven understanding of concentrated electrolytes** — •Alpha Lee

Invited Talks of the joint Symposium United Kingdom as Guest of Honor (SYUK)

See SYUK for the full program of the symposium.

SYUK 1.1	Wed	9:30–10:00	H2	**Structure and Dynamics of Interfacial Water** — •Angelos Michaelides
SYUK 1.2	Wed	10:00–10:30	H2	**A molecular view of the water interface** — •Mischa Bonn
SYUK 1.3	Wed	10:30–11:00	H2	**Motile cilia waves: creating and responding to flow** — •Pietro Cicuta
SYUK 1.4	Wed	11:00–11:30	H2	**Cilia and flagella: Building blocks of life and a physicist's playground** — •Oliver Bäumchen
SYUK 1.5	Wed	11:45–12:15	H2	**Computational modelling of the physics of rare earth - transition metal permanent magnets from SmCo$_5$ to Nd$_2$Fe$_{14}$B** — •Julie Staunton
SYUK 2.1	Wed	15:00–15:30	H2	**Hysteresis Design of Magnetic Materials for Efficient Energy Conversion** — •Oliver Gutfleisch
SYUK 2.2	Wed	15:30–16:00	H2	**Non-equilibrium dynamics of many-body quantum systems versus quantum technologies** — •Irene D'Amico
SYUK 2.3	Wed	16:00–16:30	H2	**Quantum computing with trapped ions** — •Ferdinand Schmidt-Kaler
SYUK 2.4	Wed	16:45–17:15	H2	**Breaking the millikelvin barrier in cooling nanoelectronic devices** — •Richard Haley
SYUK 2.5	Wed	17:15–17:45	H2	**Superconducting Quantum Interference Devices for applications at mK temperatures** — •Sebastian Kempf

Invited Talks of the joint Symposium Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (SYSM)

See SYSM for the full program of the symposium.

SYSM 1.1	Wed	15:00–15:30	H1	**Statics and Dynamics of Soft Wetting** — •Bruno Andreotti
SYSM 1.2	Wed	15:30–16:00	H1	**Droplets on elastic substrates and membranes - Numerical simulation of soft wetting** — •Sebastian Aland
SYSM 1.3	Wed	16:00–16:30	H1	**Wetting of Polymer Brushes in Air** — Lars Veldscholte, Guido Ritsema van Eck, Liz Mensink, Jacco Snoeijer, •Sissi de Beer
SYSM 1.4	Wed	16:45–17:15	H1	**Elastocapillary phenomena in cells** — •Roland L. Knorr
SYSM 1.5	Wed	17:15–17:45	H1	**Active contact line depinning by micro-organisms spreading on hydrogels** — Marc Hennes, Julien Tailleur, Gaëlle Charron, •Adrian Daerr

Sessions

CPP 1.1–1.12	Mon	9:30–13:00	H38	**Organic Electronics and Photovoltaics 1**
CPP 2.1–2.4	Mon	9:30–10:30	H39	**Polymer Networks and Elastomers**
CPP 3.1–3.11	Mon	9:30–12:45	H34	**Perovskite and Photovoltaics 1 (joint session HL/CPP/KFM)**
CPP 4.1–4.10	Mon	9:30–12:45	H36	**2D Materials 1 (joint session HL/CPP/DS)**
CPP 5.1–5.8	Mon	10:00–12:15	H19	**Wetting, Droplets and Microfluidics (joint session DY/CPP)**
CPP 6.1–6.7	Mon	10:30–12:45	H16	**Active Matter 1 (joint session BP/CPP/DY)**
CPP 7.1–7.8	Mon	10:45–13:00	H39	**Wetting, Fluidics and Liquids at Interfaces and Surfaces**
CPP 8.1–8.5	Mon	15:00–17:15	H38	**Focus Session: Photonic Structures from Polymer and Colloidal Self-Assembly**
CPP 9.1–9.10	Mon	15:00–17:45	H39	**Modeling and Simulation of Soft Matter (joint session CPP/DY)**
CPP 10.1–10.12	Mon	15:00–18:30	H36	**2D Materials 2 (joint session HL/CPP/DS)**
CPP 11.1–11.2	Mon	17:15–17:45	H38	**2D Materials 3 (joint session CPP/DS)**
CPP 12.1–12.80	Mon	18:00–20:00	P1	**Poster 1**
CPP 13.1–13.6	Tue	9:30–11:15	H38	**Charged Soft Matter, Polyelectrolytes and Ionic Liquid**
CPP 14.1–14.7	Tue	9:30–11:15	H39	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods**
CPP 15.1–15.8	Tue	9:30–12:00	H36	**2D Materials 4 (joint session HL/CPP/DS)**
CPP 16.1–16.11	Tue	10:00–13:00	H18	**Active Matter 2 (joint session DY/BP/CPP)**
CPP 17.1–17.41	Tue	11:00–13:00	P2	**Poster 2**
CPP 18.1–18.5	Tue	11:30–13:00	H38	**Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)**
CPP 19.1–19.5	Wed	9:30–11:00	H38	**Perovskite and Photovoltaics 2**
CPP 20.1–20.7	Wed	9:30–11:15	H39	**General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (joint session CPP/DY)**
CPP 21.1–21.7	Wed	9:30–12:05	H7	**Materials for Energy Storage (joint session KFM/CPP)**
CPP 22.1–22.10	Wed	9:30–12:30	H16	**Active Matter 3 (joint session BP/CPP/DY)**
CPP 23.1–23.9	Wed	9:30–12:00	H18	**Complex Fluids and Soft Matter 1 (joint session DY/CPP)**
CPP 24.1–24.9	Wed	9:30–12:00	H36	**2D Materials 5 (joint session HL/CPP/DS)**
CPP 25.1–25.7	Wed	11:15–13:00	H17	**2D Materials 6 (joint session DS/CPP)**
CPP 26.1–26.6	Wed	11:30–13:00	H38	**Organic Electronics and Photovoltaics 2**
CPP 27.1–27.6	Wed	11:30–13:00	H39	**Composites and Functional Polymer Hybrids**
CPP 28.1–28.8	Wed	15:00–17:15	H38	**Perovskite and Photovoltaics 3**
CPP 29.1–29.8	Wed	15:00–17:30	H15	**Biomaterials (joint session BP/CPP)**
CPP 30.1–30.4	Wed	15:00–16:00	H17	**2D Materials 7 (joint session DS/CPP)**
CPP 31.1–31.9	Wed	15:00–17:30	H18	**Active Matter 4 (joint session DY/BP/CPP)**
CPP 32.1–32.11	Wed	15:00–18:15	H34	**Perovskite and Photovoltaics 4 (joint session HL/CPP/KFM)**
CPP 33.1–33.6	Thu	9:30–11:15	H38	**Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 1**
CPP 34.1–34.3	Thu	9:30–10:15	H39	**Hydrogels and Microgels**
CPP 35.1–35.8	Thu	9:30–11:30	H17	**2D Materials 8 (joint session DS/CPP)**
CPP 36.1–36.6	Thu	10:00–11:30	H18	**Complex Fluids and Soft Matter 2 (joint session DY/CPP)**
CPP 37.1–37.8	Thu	10:30–13:00	H39	**Interfaces and Thin Films and Responsive and Adaptive Systems**
CPP 38.1–38.4	Thu	11:15–12:15	H36	**2D Materials 9 (joint session HL/CPP/DS)**
CPP 39.1–39.6	Thu	11:30–13:00	H38	**Molecular Electronics and Excited State Properties**
CPP 40.1–40.9	Thu	15:00–17:45	H38	**Organic Electronics and Photovoltaics 3**
CPP 41.1–41.8	Thu	15:00–17:30	H39	**Crystallization, Nucleation and Self-Assembly**
CPP 42.1–42.6	Thu	15:00–16:30	H31	**Perovskite and Photovoltaics 5 (joint session HL/CPP/KFM)**
CPP 43	Thu	18:00–19:00	H39	**Members' Assembly**
CPP 44.1–44.5	Fri	9:30–11:15	H38	**Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 2**
CPP 45.1–45.6	Fri	9:30–11:15	H39	**Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)**
CPP 46.1–46.9	Fri	9:30–12:00	H36	**2D Materials 10 (joint session HL/CPP/DS)**
CPP 47.1–47.11	Fri	10:00–12:45	H18	**Active Matter 5 (joint session DY/BP/CPP)**
CPP 48.1–48.4	Fri	11:30–12:30	H38	**Electrical, Dielectrical and Optical Properties of Thin Films (joint session CPP/KFM)**
CPP 49.1–49.6	Fri	11:30–13:00	H39	**Polymer and Molecular Dynamics, Friction and Rheology**
CPP 50.1–50.2	Fri	12:30–13:00	H38	**Nanostructures, Nanostructuring and Nanosized Soft Matter**
CPP 51.1–51.1	Fri	13:15–14:00	S054	**Overview Talk Claus M. Schneider (joint session O/CPP)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 H39

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

CPP 1: Organic Electronics and Photovoltaics 1

Time: Monday 9:30–13:00 Location: H38

Invited Talk CPP 1.1 Mon 9:30 H38

Ternary blend approach for boosting performance and stability of organic solar cells — •Tayebeh Ameri — University of Edinburgh, School of Engineering, Edinburgh, UK

Organic solar cells (OSCs) have now reached power conversion efficiencies over 18% on laboratory-scale devices, an important milestone towards their commercialization. The evolution in organic photovoltaic technology along with introducing non-fullerene acceptor materials and ternary blend approach caused this significant boost in the performance of solar cells.

However, for longer than a decade, when researchers were focused on boosting the power conversion efficiency of solar cells, the importance of lifetime and stability issues was overlooked by the organic photovoltaic community. Recently, more studies have been conducted and reported on the lifetime and stability of OSCs, employing different strategies to either understand the degradation mechanisms or enhance the lifetime of solar cells.

In this presentation, we overview how the ternary blend approach was developed to boost the power conversion efficiency. Moreover, we discuss how this approach can also address the stability issues related to the mostly used electron transport layer of zinc oxide and significantly increase the photostability of organic solar cells. And finally, we explain how zinc oxide must be manufactured and pretreated to avoid UV light activation, and in parallel, increase the thermal stability of the devices.

CPP 1.2 Mon 10:00 H38

Structure control during in situ printing of donor-acceptor blend films — Kerstin S. Wienhold[1], Manuel A. Reus[1], Dan Yang[1], Baojun Lin[2], Heng Zhao[2], Wei Ma[2], and •Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049 China — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

Among the next generation solar cells, in particular organic photovoltaics are gaining impact as a promising alternative to conventional silicon-based solar cells. However, despite big achievements in the last years, it remains an unresolved challenge to fabricate large-area organic solar cells without sacrificing efficiencies. The reason behind is that basic understanding is still very limited due to the complexity of the systems. Moreover, presently a substantial number of researchers use spin-coating for film fabrication, which is not compatible with the needs of a large scale production. Thus, using up-scalable fabrication methods such as printing are of immanent interest. In the present work, we use GISAXS and GIWAXS in situ during printing of donor:acceptor blends to gain fundamental understanding about the underlying film formation processes. Different examples of polymer donors and small molecule acceptors are presented and the resulting morphologies are correlated with solar cell device performance.

CPP 1.3 Mon 10:15 H38

Revealing the Thermally Induced Degradation of PM6:Y6 based Bulk Heterojunction Organic Solar Cell — •Shahidul Alam, Hua Tang, Maryam Alqurashi, Wejdan Althobaiti, Si Chen, Haya Aldosari, Jafar I. Khan, and Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia

Thermally-induced degradation in bulk-heterojunction OSCs is an obvious barrier to the fabrication of stable devices. Thus, practical approaches and strategies need to be identified their inherent thermal instability. In this work, the thermally induced degradation of the most commonly used system PM6:Y6 is investigated by varying temperatures and different exposure conditions. The degradation pathways have been identified by applying several opto-electrical and spectroscopic characterizations methods. Due to the reduced charge carrier mobility and extraction probability, the thermally degraded device exhibits significant losses in the VOC and FF. Furthermore, the field dependence of charge generation, charge extraction, photo-generated charge density, and charge recombination dynamics in solar cells were studied by the TDCF optical-pump electronic-probe technique. By using all the analyses, we can explain the significant recombination process that dominates device performance and thermal stability. Finally, device simulation by SETFOS of the JV characteristics was used to confirm experimentally determined thermally induced degradation.

CPP 1.4 Mon 10:30 H38

Developing the next generation of photovoltaics with high efficiencies — •Elisabeth Erbes[1,2], Matthias Schwartzkopf[1], Constantin Harder[1,3], Susann Frenzke[1], Benedikt Sochor[1], Naireeta Biswas[1,2], Stephan V. Roth[1,4], and Simone Techert[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Institute for X-ray Physics, Goettingen University, Goettingen, Germany — [3]Technical University of Munich, Munich, Germany — [4]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

A crucial challenge in bio-inspired energy research is to develop a rationale for the synthesis and use of sustainable, bio-based materials. Cellulose fibers have excellent mechanical strength, are thermally stable, are very lightweight and have a very low surface roughness in thin films. On the other hand, the use of small molecules in OSC is well known to increase the power conversion efficiency. The idea is to combine the use of cellulose and small molecules to create a sustainable organic solar cell with high efficiencies. The current study aims to investigate systematically the OSC matrix PM6:Y6 doped with optical-light absorbing, electron transfer (ET) dyes. The structural and morphological integrity of the dyes were studied with grazing incidence small angle and wide angle X-ray scattering techniques (in situ GISAXS and static GIWAXS) and photo-sensitization experiments. This analysis showed us the intercalation dynamics, distribution and function of pyrene-based photo-dopants within the PM6:Y6 matrix and whether these dopants alter the overall polymer structures.

CPP 1.5 Mon 10:45 H38

Ultrafast charge carriers separation at organic donor-acceptor interfaces - Influence of molecular vibrations — •Maximilian F. X. Dorfner[1], Sebastian Hutsch[1], Raffaele Borrelli[2], Maxim F. Gelin[3], and Frank Ortmann[1] — [1]Department of Chemistry, Technische Universität München, 85748 Garching b. München (Germany) — [2]DISAFA, University of Torino, Largo Paolo Braccini 2, I-10095 Grugliasco (TO), Italy — [3]School of Sciences, Hangzhou Dianzi University, Hangzhou 310018, China

In this work the charge transfer dynamics of photogenerated excitons at a donor-acceptor interface of an organic solar cell blend is examined. This is done by means of a fully quantum mechanical treatment of an effective Holstein model including the relevant electronic orbitals coupled to over one hundred vibrational modes, parametrized by density functional theory calculations. To solve this coupled electron-phonon system we make use of the numerically quasi-exact matrix-product-state ansatz. We find that, depending on the driving energy, different mechanisms are predominantly responsible for the charge separation at the interface. For near zero driving the ultrafast electron transfer is prevalently due to kinetic processes, while at larger driving the separation of carriers can be traced back to dissipative phonon emission connected with the dominant molecular vibrations. This charge transfer picture is consistent with a novel semi-classical hopping approach, with which we compare. These results show that dissipation of energy to the phonon is essential for charge separation for systems with a moderate driving force.

CPP 1.6 Mon 11:00 H38

Revealing the formation kinetics of the active layer for non-fullerene organic solar cells — •Xinyu Jiang[1], Suo Tu[1], Manuel A. Reus[1], Julija Reitenbach[1], Christian L. Weindl[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]DESY, Notkestraße 85, 22607 Hamburg

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. In addition, it is difficult to observe the structure formation process of the active layer during deposition, which is crucial for gaining a fundamental understanding. 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. In this work, we fabricate an active layer, which contains a donor polymer (PDTBT2T-FTBDT) and a non-fullerene acceptor (BTP-4F) with a slot-die coating. The structure formation of the polymer domains kinetics 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 drying of non-fullerene organic BHJ thin films.

15 min. break

CPP 1.7 Mon 11:30 H38

Re-evaluation of Published Figures of Merit and Introduction of Novel figure of merit for Transparent Conducting Electrodes used in Photovoltaics — •Aman Anand[1,2], Md Moidul Islam[1,2], Rico Meitzner[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

Transparent conductive electrodes (TCEs) are one of the important components of photovoltaic technologies. Since they are transparent and conductive, they allow light to enter the device and the photocurrent generated to be drawn into the outer electric circuit. In theory, TCEs should have the highest light transmission and conductivity. Both traits, however, must be balanced. The selection of the best TCE depends on the photovoltaic material system and is evaluated using so-called figures-of-merit (FOM). A novel and exact FOM is presented here that explicitly analyzes the impact on photovoltaic performance. This novel and exact FOM has several important properties, including i) proportionality to the solar device's potential power output, ii) normalization to the theoretically ultimately attainable photovoltaic performance, and, thus, iii) significant direction for the development of advanced TCEs. This work reassesses and compares a variety of realized state-of-the-art semitransparent electrodes.

CPP 1.8 Mon 11:45 H38

Cycling stability of cellulose-based electronics — •Stephan V. Roth[1,2], Calvin J. Brett[1,2], Ola K. Forslund[1], Elisabetta Nocerino[1], Lucas P. Kreuzer[3], Lionel Porcar[4], Norifumi L. Yamada[5], Martin Mansson[1], Peter Müller-Buschbaum[3], and L. Daniel Söderberg[1] — [1]KTH Royal Institute of Technology, SE-10044 Stockholm — [2]DESY, D-22607 Hamburg — [3]TU München, Physik-Department, Lehrst. f. Funktionelle Materialien, D-85748 Garching — [4]ILL, F-38042 Grenoble — [5]KEK, Tokai (JPN)

In organic electronics, hybrid materials combining high-strength biomaterials and conducting organic polymers allow for disentangling mechanical flexibility and functionality. Yet, degradation in such complex organic electronics applications is still less addressed. We thus combine sprayed cellulose nanofibrils (CNF) templates due to their hierarchical, nanoporous morphology and a conductive polymer blend poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) to correlate the impact of cyclic relative humidity changes with device performance and nanostructure evolution. The conductivity of the CNF/PEDOT:PSS hybrid shows reversible changes: The PEDOT:PSS blend undergoes cyclic wetting/dewetting on the CNF backbone accompanied by swelling and deswelling of PEDOT:PSS moieties in the pores. The cycling stability of the device performance is ensured by reversible rearrangement of the CNF backbone. With CNF acting as structural reinforcing template, interestingly, no macroscopic swelling is observed, proving the applicability in e.g. supercapacitors.

CPP 1.9 Mon 12:00 H38

Dual-Gate Organic Electrochemical Transistors and Circuits — •Hsin Tseng, Anton Weissbach, Karl Leo, and Hans Kleemann — Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Dresden, Germany

Organic mixed ionic-electronic conductors (OMIECs) are currently in the spotlight of research for diverse applications. Among all, organic electrochemical transistors (OECTs) stand out as organic synaptic devices for integrated bioelectronics leading to neuromorphic computing applications, thanks to their low operating voltage, biocompatibility, and the ionic and electronic interactions in OMIECs. Modifying OMIECs by molecular design enables accumulation-mode OECTs, resulting in broad IC applications. However, the side chain molecular design of the polymer is unfavorable for IC design and manufacturing processes. Here, we show an OECT with photo-patternable solid electrolyte advancing towards integrated circuits. We discuss how alterable device parameters can be employed to adjust the OECT performance. In particular, we demonstrate how the biasing conditions govern the time constant of OECTs. In addition, we discuss how a dual-gate OECT architecture can be employed to tune the threshold voltage of OECTs and control the ionic and electronic charge transport in the electrolyte and OMIECs without any complicated molecular design. The electrical analysis of solid-state electrolyte OECTs provides new insights stimulating higher investigations on ionic and electronic interactions and coupled transport properties in OMIECs and paves the foundation for the integration of OECTs for advanced applications.

CPP 1.10 Mon 12:15 H38

Design of Monolithic All-Organic Oxygen Sensors — •Toni Bärschneider and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden

Organic electronic devices, such as light-emitting diodes (OLEDs) and photodetectors (OPDs), are ideal for sensor application because of their versatility and flexibility. Additionally, they can be easily fabricated on any substrate, making monolithic sensor application possible. This allows for an easy miniaturization and a cheap fabrication. Organic room temperature phosphorescence (RTP) materials are well suited for optical oxygen sensors because of their strong oxygen dependency.

In this work, we developed a monolithic all-organic oxygen sensor which is composed a RTP sensing layer, an ultraviolet OLED as excitation source, and a novel narrow bandwidth OPD for detection. The RTP sensing layer shows fluorescence and phosphorescence at room temperature at the same time which enables self-referencing to avoid photodegradation-caused distortion. Due to the long phosphorescence lifetime, sensing withing the ultra-trace range is possible.

The presented sensors overcome drawbacks of common optical oxygen sensors such as complexity, expensive read-out electronics, and a lack of possible miniaturization.

CPP 1.11 Mon 12:30 H38

Towards all solution-processed OFETs using microcontact printed electrodes — •Kirill Gubanov[1], Manuel Johnson[1], Melda Akay[1], Kim Thomann[1], Dan Shen[1,2], Xing Cheng[2], and Rainer H. Fink[1] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]South University of Science and Technology, Shenzhen, China

Printed electronics is expected to facilitate low-cost solvent prepared devices for potential applications in RFID, flexible displays, OLEDs and transistors. Furthermore, microcontact printing may be used in a large-scale production using roll-to-roll printing with direct access to structures on the micrometer level. The preparation of the microstructured conductive electrodes using PEDOT:PSS ink for applications in OFETs was successful in various aspects: the electrodes were fabricated with very good structural definition and high reproducibility on solvent-prepared 2D-extended single-crystalline C8-BTBT films. A defined mechanical load of the PDMS stamps pre-treated with O2 plasma yielded good structural quality and competitive electrical performance. In particular, the implementation of the MWCNTs in the PEDOT:PSS ink has a direct impact on the charge carriers transport efficiency, leading to the contact resistance decrease. In addition to electrical characterization made with KPFM and IV-curves, the morphology and structure analysis was performed using VLM, AFM and 3D Microscopy, providing with an insight into the structural quality of the contacts and relate their structures to the overall device performances. The research is funded by the BMBF (contract 05K19WE2).

CPP 1.12 Mon 12:45 H38

Effect of trap states on the performance of organic photodetectors — •Jakob Wolansky[1], Sebastian Hutsch[2], Felix Talnack[1], Michel Panhans[2], Jonas Kublitski[1], Stefan Mannsfeld[1], Frank Ortmann[2], Johannes Benduhn[1], and Karl Leo[1] — [1]Technische Universität Dresden, Dresden, Germany —

[2]Technische Universität München, Garching b. München, Germany

Due to the broad range of modern applications, the demand for photodetectors is drastically increasing, and in particular, organic photodetectors (OPDs) can meet the diverse requirements. However, the specific detectivity of OPDs is significantly below the thermal limit and is currently restricted by the high noise spectral density. Kublitski *et al.*[1] recently showed that the shot noise and hence the dark current (J_D) dominates the noise spectral density at negative bias. Further, the authors suspect that mid-gap trap states cause the high J_D.

Here, we study devices with a well-performing absorber layer without an electron acceptor and, therefore, we do not expect any charge-transfer states to form. Nevertheless, we can observe sub-bandgap absorption in ultra-sensitive external quantum efficiency measurements. By utilizing different device processing parameters and employing different interface layers, we identify the origin of these sub-bandgap excitations. Interestingly, we observe a clear correlation between the device performance and the presence and quantity of trap states. The relation between molecular structure and device performance gives a new direction for reducing J_D further in OPDs and improving their specific detectivity. [1] Kublitski, J. *et al.* Nat Commun 12, 551 (2021)

CPP 2: Polymer Networks and Elastomers

Time: Monday 9:30–10:30 Location: H39

CPP 2.1 Mon 9:30 H39

The non-ideal preparation state of polymer (model) networks — •Michael Lang[1] and Toni Müller[1,2] — [1]Institut Theorie der Polymere, Leibniz Institut für Polymerforschung Dresden, Hohe Straße 6, 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Zellescher Weg 17, 01069 Dresden, Germany

We demonstrate that the phantom modulus can be split into two major contributions: the cycle rank of the active network structure and a correction resulting predominantly from non-ideal chain conformations at the instance of cross-linking. The correction contains several contributions related to loop formation, an effective repulsion between network junctions, and an excess strain of chains that develops towards the end of the reactions, if reaction partners become sparse. This challenges the text-book assumption that network strands are incorporated into the network with the same conformations as a free chain inside the reaction container. Our results are relevant for developing a better understanding of rubber elasticity and its dependence on the network formation process.

CPP 2.2 Mon 9:45 H39

Nonlinear elasticity under constraints and predeformations: a group theoretical approach — •Segun Goh[1,2], Hartmut Löwen[2], and Andreas M. Menzel[3] — [1]Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Heinrich-Heine Universität Düsseldorf, 40225 Düsseldorf, Germany — [3]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany

The mechanical response of elastic materials frequently involves predeformations. Moreover, if an active or driven material is exposed to an external condition, a mismatch between the activity/driving and external condition may lead to a hidden predeformation in the system in its mechanical equilibrium state. Then the assumption of linear response breaks down, making descriptions of nonlinear elasticity compulsory even if the applied deformation is infinitesimally small. In this talk, we discuss how to develop a theoretical framework to meet this challenge and thereby, to address elasticity consistently for both small and large deformations. Specifically, employing concepts from group theory and Lie algebra, we suggest an idea to construct finite deformation gradients from infinitesimal group generators. Generalized nonlinear shear deformations and elastic moduli are defined subsequently. Possible applications will also be discussed.

CPP 2.3 Mon 10:00 H39

Surface structure and rheology of amphiphilic co-polymer networks on different length scales — •Kevin Hagmann[1], Nora Fribiczer[2], Sebastian Seiffert[2], Carolin Bunk[3], Frank Böhme[3], and Regine von Klitzing[1] — [1]Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt — [2]Department of Chemistry, Johannes Gutenberg University Mainz, D-55128 Mainz — [3]Leibniz-Institut für Polymerforschung Dresden e.V., D-01069 Dresden

This study focuses on the relation between structure, swelling abilities and mechanical/rheological properties of films of amphiphilic copolymer networks (ACNs). First, the correlation between different synthesis strategies for gel films and their resulting properties will be described. Secondly, the effect of solvents of different polarity on the swelling ability will be presented on different length scales. For this purpose, topology and near surface structure are studied with atomic force microscopy (AFM) and grazing incidence small angle x-ray scattering (GISAXS), respectively. We also put special emphasis on the determination of mechanical and rheological properties laterally and orthogonally to the gel surface by carrying out dynamic AFM indentation experiments. In order to evaluate heterogeneities the mechanical and rheological behaviour at the interface of the ACNs will be presented on various length scales (nm - μm). The study shows that the synthesis strategy has a strong effect on the gel structure and on nano/microrheological properties. The structure and rheology of gel films will be compared with results obtained of the respective bulk gel.

CPP 2.4 Mon 10:15 H39

Correlations of infrared spectroscopy and DSC measurements to determine the yield of scission under irradiation in biopolyesters — •David Krieg, Mirko Rennert, and Michael Nase — Institut für Biopoylmerforschung der Hochschule für Angewandte Wissenschaften Hof

Under the influence of ionizing irradiation, biopolyesters can either undergo crosslinking or scissioning. It was shown that the yield of corsslinking for polyesters such as polybutylenadipat-terephthalat (PBAT) can be correlated to changes in peaks in the IR spectrum and the onset time of the melting peak while heating during DSC measurements using the Avrami equation [Kijchavengkul 2008]. For biopolyesters such as polyhydroxybutyrate (PHB) and polylactic acid (PLA) sicsioning is the dominant process under irradiation. This talk will go into detail, whether similar correlations as seen in crosslinking PBAT can be found in PLA and PH3B, when scission is the dominate reaction and what structural changes in the polymer make this correlation possible.

CPP 3: Perovskite and Photovoltaics 1 (joint session HL/CPP/KFM)

Time: Monday 9:30–12:45 Location: H34

CPP 3.1 Mon 9:30 H34

The Electronic Structure of $Cs_2AgBiBr_6$ at Room Temperature — •Julian Gebhardt[1,2] and Christian Elsässer[1,2,3] — [1]Fraunhofer Institute for Mechanics of Materials IWM, 79108 Freiburg — [2]Cluster of Excellence livMatS at FIT - Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-University Freiburg, 79104 Freiburg — [3]Freiburg Materials Research Center (FMF), Albert-Ludwigs-University Freiburg, 79104 Freiburg

$Cs_2AgBiBr_6$ is a stable halide double perovskite with a band gap of about 2.2 eV. Therefore, it is intensively studied as possible lead free alternative to hybrid perovskite solar cell absorber materials such as methylammonium-lead iodide. However, power conversion efficiencies of solar cells with this material have not yet exceeded 3%. A detailed understanding of the electronic structure of this material is difficult, due to the variance of reported data and experimental as well as theoretical difficulties that occur in going beyond a qualitative understanding of such an indirect semi-conductor at device operation temperature. Here we combine self-energy corrected electronic-structure theory including spin-orbit coupling and structural dynamics at room temperature to model and understand this compound in a quantitative manner, and we compare our theoretical findings with experimental ones. Based on an achieved good agreement, we propose that the observed low power conversion efficiencies can be attributed to the density of states in the conduction band region. From the relation between dimensionality and electron conductivity, we suggest a general design principle for absorber material search.

CPP 3.2 Mon 9:45 H34

Photon-echo spectroscopy of a $CH_3NH_3PbI_3$ perovskite single crystal — •Stefan Grisard[1], Artur V. Trifonov[1,2], Aleksandr N. Kosarev[1,3], Ilya A. Akimov[1,3], Dmitrii R. Yakovlev[1,3], Julian Höcker[4], Vladimir Dyakonov[4], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund — [2]Spin Optics Laboratory, St. Petersburg State University, Russia — [3]St. Petersburg, Russia — [4]Experimental Physics 6, Julius-Maximilian University of Würzburg

Lead halide perovskites such as $CH_3NH_3PbI_3$ (MAPbI$_3$) show outstanding characteristics important for photovoltaic and optoelectronic applications. However, the peculiarities of light-matter interactions in these materials are far from being fully explored. Here, we applied time-resolved photon echo spectroscopy to a high quality MAPbI$_3$ single crystal highlighting the importance of inhomogeneous broadening of excitonic transitions even at cryogenic temperatures. Furthermore, we developed an experimental photon-echo polarimetry method that unambiguously identifies contributions from exciton and biexciton to the coherent optical response. Most importantly, our method allows to accurately extract the biexciton binding energy of 2.4meV, even though the period of the observed quantum beats exceeds the coherence times of exciton and biexciton.

CPP 3.3 Mon 10:00 H34

Structural properties of (hot-)pressed MAPbI$_3$ films revealed by detailed temperature-dependent optical analyses — •Christina Witt[1], Konstantin Schötz[1], Nico Leupold[2], Simon Biberger[1], Philipp Ramming[1], Ralf Moos[2], and Fabian Panzer[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth 95440, Germany — [2]Department of Functional Materials, University of Bayreuth, Bayreuth 95440, Germany

Halide perovskites attracted much attention in recent years, due to the remarkable increase in corresponding solar cell efficiencies. More recently, hot-pressing has emerged as attractive method for manufacturing and post-treatment of perovskite films [1, 2]. However, a detailed understanding regarding the role of temperature during hot-pressing on resulting film properties is still missing. Thus, we use temperature-dependent PL and absorption measurements of MAPbI$_3$ thin films pressed with different temperatures and in detail analyze their optical properties. This allows us to draw conclusions about structural and optoelectronic properties, revealing that an increased temperature improves film morphology, structural and optoelectronic film properties.

[1] Witt, C. et al. Impact of Pressure and Temperature on the Compaction Dynamics and Layer Properties of Powder-Pressed Methylammonium Lead Halide Thick Films. ACS Appl. Electron. Mater. 2020, 2 (8), 2619-2628.

[2] Pourdavoud, N. et al. Room-Temperature Stimulated Emission and Lasing in Recrystallized Cesium Lead Bromide Perovskite Thin Films. Adv. Mater. 2019, 31, 1903717.

CPP 3.4 Mon 10:15 H34

Application of atomic layer deposition and x-ray photoelectron spectroscopy in perovskite solar cells — •Małgorzata Kot[1], Chittaranjan Das[2], Lukas Kegelmann[3], Hans Koebler[3], Mikhailo Vorokhta[4], Carlos Escudero[5], Steve Albrecht[3], Antonio Abate[3], and Jan Ingo Flege[1] — [1]BTU Cottbus-Senfteberg, Cottbus, Germany — [2]KIT, Eggenstein-Leopoldshafen, Germany — [3]HZB, Berlin, Germany — [4]Charles University, Prague, Czech Republic — [5]ALBA Synchrotron, Cerdanyola del Vallès, Spain

In this work we have utilized near-ambient pressure and ultra-high vacuum X-ray photoelectron spectroscopy as well as atomic layer deposition to investigate perovskite solar cells (PSCs). We have demonstrated that ultrathin room temperature atomic layer-deposited aluminium oxide on the perovskite surface very effectively suppresses iodine migration[1] and improves the long term stability and efficiency of PSCs [2,3]. Furthermore, exposure to light proves more detrimental to the perovskite film than exposure to water vapor.[2] Absorbed photons create Frenkel defects in the perovskite crystal and their number strongly depends on the used illumination. The higher the photon flux, the higher the concentration of Frenkel defects, and thus the stronger the degradation of power conversion efficiency and the stronger the hysteresis in the J-V characteristics. [1] C. Das, M. Kot et al., Cell Reports Physical Science 2020, 1, 100112. [2] M. Kot et al., ChemSusChem 2020, 13, 5722. [3] M. Kot et al., ChemSusChem 2018, 11, 3640.

CPP 3.5 Mon 10:30 H34

Chemical Engineering of Ferroelastic Twin Domains in MAPbI3 Thin Films — •Yenal Yalcinkaya[1], Ilka Hermes[1], Tobias Seewald[2], Katrin Amann-Winkel[1], Lothar Veith[1], Lukas Schmidt-Mende[2], and Stefan A.L. Weber[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, University of Konstanz, Universitätsstr. 10, 78464, Germany

In this study, we introduce a new chemical method for controlling the strain in methylammonium lead iodide (MAPbI3) perovskite crystals by varying the ratio of Pb(Ac)2 and PbCl2 in the precursor solution. We used a combination of piezoresponse force microscopy (PFM) and X-ray diffraction (XRD) to observe the effect on crystal strain. We observed larger ferroelastic twin domains upon increasing the PbCl2 content, indicating increased crystal strain via PFM images. We confirmed the increased crystal strain via the XRD patterns with strong crystal twinning features. We suggest that this behaviour is caused by different evaporation rates of methylammonium acetate and methylammonium chloride which led to a strain gradient during the crystallization as revealed by time-of-flight secondary ion mass spectroscopy (ToF-SIMS) and grazing incidence x-ray diffraction (GIXRD) measurements. We observed films with larger twin domain structures show an increased carrier via time-resolved photoluminescence (TRPL). The results demonstrate the potential of chemical strain engineering as an easy method for controlling strain-related e*ects in lead halide perovskites.

CPP 3.6 Mon 10:45 H34

Inspecting the local structure of cubic phase halide perovskites from first-principles — •Xiangzhou Zhu, Sebastián Caicedo-Dávila, Christian Gehrmann, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Halide perovskites (HaPs) have been identified as one of the most promising optoelectronic materials in recent years. Different from the conventional inorganic semiconductors, HaPs exhibit profound deviations from their average atomic structure at finite temperature, which have important consequences for their optoelectronic properties. However, a detailed understanding of these local structural fluctuations, the underlying physical mechanisms as well as their consequences is far from complete. Here, we perform molecular dynamics (MD) calculations based on density functional theory (DFT) to investigate the local structure and anharmonic dynamics of $CsPbBr_3$ in the cubic phase at T=425 K and 525K. We find that motions of neighboring Cs-Br atoms interlock within a nominal cubic unit cell. This manifests in the most likely Cs-Br distance being significantly shorter than what is inferred from an ideal cubic structure. Furthermore, we use the statistical information on the dynamic atomic distributions to quantify the effective potential associated with certain atomic motions at two temperatures. We find that Br motions occur in a dynamically disordered potential energy landscape and relate the Cs motion as well the Cs-Br coupling to $PbBr_6$ octahedral rotations.

30 min. break

CPP 3.7 Mon 11:30 H34

Distinct Resonances in Absorption Spectra of Lead Halide-based Quantum Dots — •Anja Barfüsser, Quinten A. Akkerman, Sebastian Rieger, Amrita Dey, Ahmet Tosun, Tushar Debnath, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Nano-Institute Munich and Department of Physics, Ludwig-Maximilians-Universität (LMU), Königinstr. 10, 80539 Munich, Germany

In recent years, perovskite nanocrystals have attracted much attention for their unique optical properties. Here, we discuss sphere-like lead halide-based quantum dots with diameters in the range of 4.5-12 nm featuring a multitude of distinct resonances in their absorption spectra. We have investigated the nature of these resonances by comparing experimental data with model calculations based on weak and strong confinement. In transient absorption experiments, bleaching and induced absorption signals are observed, which we discuss in terms of confined excitons and biexcitonic contributions.

CPP 3.8 Mon 11:45 H34

Revealing the doping density in perovskite solar cells and its impact on device performance — •Francisco Peña-Camargo and Martin Stolterfoht — Physik weicher Materie, Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14776 Potsdam, Germany

Inorganic semiconductors can be electronically doped with high precision. Conversely, there is still conjecture regarding the assessment of the electronic doping density in metal-halide perovskites, not to mention of a control thereof. This study presents a multifaceted approach to determine the electronic doping density for a range of different lead-halide perovskite systems. Optical and electrical characterisation techniques comprising intensity-dependent and transient photoluminescence, AC Hall effect, transfer-length-methods, and charge extraction measurements were instrumental in quantifying an upper limit for the doping density. The obtained values are subsequently compared to the electrode charge per cell volume at short-circuit conditions (CU_{bi}/eV), which amounts to roughly 10^{16} cm^{-3}. This figure of merit represents the critical limit below which doping-induced charges do not influence the device performance. The experimental results demonstrate consistently that the doping density is below this critical threshold ($< 10^{12}$ cm^{-3} which means $\ll CU_{\mathrm{bi}}/eV$) for all common lead-based metal-halide perovskites. Nevertheless, although the density of doping-induced charges is too low to redistribute the built-in voltage in the perovskite active layer, mobile ions are present in sufficient quantities to create space-charge-regions in the active layer.

CPP 3.9 Mon 12:00 H34

Ground-state structures, electronic structure, transport properties and optical properties of anion-ordered anti-Ruddlesden-Popper phase oxide perovskites — •Dan Han, Shizhe Wang, Thomas Bein, and Hubert Ebert — Department Chemie, Ludwig-Maximilians-Universität München, Germany

Anti-Ruddlesden-Popper (ARP) phase oxide perovskites Ca4OA2 (A = P, As, Sb, Bi) have recently attracted great interest in the field of ferroelectrics and thermoelectrics, while their optoelectronic application is dominantly limited by their indirect band gaps. In this work, we consider A-site anion ordering in Ca4OA2 (A = P, As, Sb, Bi), and find that it induces an indirect-to-direct band gap transition. Using first-principles calculations, we study the ground-state structures, electronic structure, transport properties and optical properties of anion-ordered ARP phase oxide perovskites Ca4OAA'. Based on an analysis of the lattice dynamics, the ground-state structures of Ca4OAsSb, Ca4OAsBi, Ca4OPSb and Ca4OPBi are identified. In contrast to the Ruddlesden-Popper (RP) phase oxide and halide counterparts, Ca4OAA' show larger band dispersion along the out-of-plane direction, smaller band gaps and highly enhanced out-of-plane mobilities, which is ascribed to the short interlayer distances and enhanced covalency of the pnictides. Although the out-of-plane mobilities of these n = 1 ARP phase perovskites highly increase, comparatively strong polar optical phonon (POP) scattering limits the further enhancement of their mobilities. This work shows that these anion-ordered Ca4OAA' exhibit the potential for optoelectronic applications.

CPP 3.10 Mon 12:15 H34

Including light management concepts in performance prediction modelling of perovskite-silicon tandem solar cells by implementing transfer matrix method — Aminreza Mohandes[1,2], Peymaneh Rafieipour[1,2], Mohammad Moaddeli[1], and •Mansour Kanani[1] — [1]Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran — [2]Department of Physics, Shiraz University, Shiraz, Iran

The 2-T monolithic perovskite-silicon tandem design holds a record efficiency of 29.80%, recently. To perform more accurate, complete and experimentally reliable modelling of tandem solar cell, we adopt the transfer matrix method (TMM) which incorporates the interfacial reflections, light scattering and parasitic absorption losses in the calculation of the light transmitted from the top perovskite solar cell. The results reveal that the light scattering and interfacial reflection losses cannot be ignored and the previously used Beer-Lambert exponential relation is insufficient for studying tandem configuration. Including TMM method in the performance optimization of the tandem solar cells lets to consider light management concepts more extensively. Therefore, identifying and reducing optical losses in each layer/interface and designing appropriate anti-reflection coatings in a multilayer tandem simulation can be achieved. In this study, standalone and tandem devices have been analyzed and the effect of absorber layer thickness variation, J-V curves, external quantum efficiency (EQE), filtered spectra, current matching, and tandem performance parameters on the cell efficiency is considered.

CPP 3.11 Mon 12:30 H34

Highly Efficient Perovskite-on-Silicon Tandem Solar Cells on Planar and Textured Silicon — •Christian M. Wolff[1], Xin Yu Chin[2], Kerem Artuk[1], Deniz Türkay[1], Daniel Jacobs[1], Quentin Jeangros[2], and Christophe Ballif[1,2] — [1]École polytechnique fédérale de Lausanne, STI IEM PVLAB, Rue de la Maladière 71b, 2000 Neuchâtel — [2]Centre Suisse d'Electronique et de Microtechnique, Rue Jaquet-Droz 1, 2002 Neuchâtel

Multi-junction devices offer the possibility to harness the sun's light beyond the limitations of single-junction solar cells. Among the different combinations perovskite-on-silicon (Pk/Si) tandems hold the great promise of high efficiencies >30%, while maintaining low cost. I will report on our latest progress in the development of Pk/Si tandems comparing our efforts on single-side and double-side textured Pk/Si tandems, reaching a V_{OC} up to 1.95V, summed short-circuit currents above $41\mathrm{mA/cm}^2$, and certified efficiencies >29%, on an active area of $1\mathrm{cm}^2$. We achieved these results by dedicated electrical and optical optimizations of all layers within the stack. Specifically, we reduced recombination and transport losses in the Pk absorbers through process and additive engineering for both solution-processed one-step and hybrid two-step deposited Pks, and improved the transparency of the front stack electrodes and contacts through simulation-guided optimizations of the front grid and layer thicknesses. Furthermore, we investigated the stability of single-junction Pk and tandem devices under reverse-bias and standardized accelerated aging conditions.

CPP 4: 2D Materials 1 (joint session HL/CPP/DS)

Time: Monday 9:30–12:45 Location: H36

Invited Talk CPP 4.1 Mon 9:30 H36

g-factors in van der Waals heterostructures: revealing signatures of interlayer coupling — •Paulo E. Faria Junior — University of Regensburg, Regensburg, Germany

The interplay of the spin and the orbital angular momenta of electrons in semiconductors governs the observed Zeeman splitting, often described by the effective g-factors. In the realm of 2D materials, transition metal dichalcogenides (TMDCs) are ideal candidates to explore the manifestation of coupled spin and orbital degrees of freedom under external magnetic fields. In this talk, I will cover the basic physics behind the Zeeman splitting and effective g-factors, emphasizing the recent first-principles developments in monolayer TMDCs that nicely reproduce the available experimental data. These new theoretical insights demystify the valley-Zeeman physics in TMDCs and finally establish a connection to the vast existing knowledge in the area of III-V materials. Beyond monolayers, I will discuss TMDC-based van der Waals heterostructures, particularly MoSe2/WSe2 and WS2/graphene systems, in which the spin-valley physics and g-factors encode valuable information about the interlayer coupling.

CPP 4.2 Mon 10:00 H36

Optical Properties of Encapsulated Transition-Metal Dichalcogenide Monolayers, Bilayers, and Heterostructures — •Manan Shah[1], Philip Klement[1], Sangam Chatterjee[1], Kyungnam Kang[2], Eui-Hyeok Yang[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany — [2]Department of Mechanical Engineering, Stevens Institute of Technology, Hoboken, NJ, 07030, USA

Van-der-Waals heterostructures (vdW-HSs) based on 2D-layered materials have received unrivaled attention among nanomaterials due to their promising optoelectronic properties induced by moiré potential landscapes; secondly, their strong light-matter interactions; and third, the promise of bandgap engineering capabilities. The optical properties of transition-metal dichalcogenides (TMDs) depend considerably on the substrate, stacking configuration, interface quality, and encapsulation. As more and more layered materials have come into the focus, the demand for a comprehensive understanding of their optical, optoelectronic, and vibronic properties is increasing drastically.

We focus on the discussion of photoluminescence and the Raman response of tungsten-based TMD monolayers and stacks thereof [1, 2], as well as encapsulated configurations. We further aim at unraveling structural alterations and emission properties by monitoring the temporal behavior in their responses. [1] Semiconductors 2019, 53, 2140. [2] Sci. Rep. 2022, 12, 6939.

CPP 4.3 Mon 10:15 H36

Electrically Tunable Photoluminescence in Monolayer MoS_2 and graphene/MoS_2 Heterostructures — •Tarlan Hamzayev and Giancarlo Soavi — Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany

The optical response of monolayer (ML) transition metal dichalcogenides (TMDs) is dominated by the co-existence, even at room temperature, of excitons, bi-excitons, and trions.

The photoluminescence (PL) emission of these quasi-particles can be modulated via external knobs, such as doping, pressure and strain. In particular, the PL emission from the neutral exciton is greatly modulated during the crossover from the undoped to the highly doped regime [1]. In the latter case, PL emission is mainly suppressed due to the presence of trions, which have a fast non-radiative decay.

In this work, we study the gate dependence of the PL emission in encapsulated ML MoS_2 and ML graphene/MoS_2 heterostructures (HS). We show that in the HS region the PL emission mainly comes from neutral excitons even at large values of external gate voltage, thus confirming that graphene is an efficient filter for PL emission [2]. This work clarifies the interplay between charge transfer and PL filtering in graphene/TMD layered HS.

[1] Mak, K. F. et al. Nature materials 12, 207-211 (2013).

[2] Lorchat, E. et al. Nature Nanotechnology 15, 283-288 (2020).

15 min. break

CPP 4.4 Mon 10:45 H36

Integration of Transferable Organic Semiconductor Nanosheets with 2D Materials for van der Waals Heterojunction Devices — •Sirri Batuhan Kalkan[1], Emad Najafidehaghani[2], Ziyang Gan[2], Fabian Alexander Christian Apfelbeck[1], Uwe Hübner[3], Antony George[2], Andrey Turchanin[2], and Bert Nickel[1] — [1]Faculty of Physics and CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 Munich, Germany — [2]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, Lessingstr. 10, 07743, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Albert-Einstein-Str. 9, 07745, Jena, Germany

Evaporation of organic semiconductors (OSC) on atomically thin transition metal dichalgonides (TMD) for van der Waals (vdW) heterojunctions is limited by obstructed growth of the organic small molecules on the TMD surface. For the realization of such vdW heterojunction devices, we have established a transfer technique that allows for wafer-scale fabrication of 50 nm OSC nanosheets on TMDs. A key feature of this transfer is the controlled release of the ultrathin OSC film from a water-soluble sacrificial film by a suited wetting geometry. We demonstrate functional and highly ordered OSC nanosheets on prefabricated electrodes and TMD monolayers. Devices fabricated this way include unipolar, ambipolar and anti-ambipolar field-effect transistors [1].

References: [1] Kalkan et al., Wafer scale synthesis of organic semiconductor nanosheets for van der Waals heterojunction devices, npj 2D Materials and Applications 5, 92 (2021)

CPP 4.5 Mon 11:00 H36

Non-resonant and resonant low-frequency Raman scattering in twisted TMDC bilayers at millikelvin temperatures — •Hendrik Lambers[1], Nihit Saigal[1], Torsten Stiehm[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Twisted TMDC bilayers are subject of many current studies because they can host many body physics and correlated phases such as superconductors and Mott insulators.[1] The moiré potential evolving with a twist angle or lattice constant mismatch could also be exploited to simulate Mott-Hubbard physics. The interlayer coupling within the bilayer correlates with the interlayer breathing mode and the shear mode, which can be characterized by low frequency Raman spectroscopy.[2] We study TMDC heterobilayers of WSe2 and MoSe2 by resonant and non-resonant Raman spectroscopy at millikelvin temperatures. The shear mode is resonant with the exciton transitions in both monolayers and its lineshape and transition energy are modified due to coupling to the exciton continuum. In addition, several sharp and highly resonant modes are observed in the high frequency Raman spectrum. We acknowledge financial support via DFG WU 637/7-1 and SPP2244. [1] L. Sigl et al., Phys. Rev. Research 2, 042044(R) (2020) [2] J. Holler et al., Appl. Phys. Lett. 117, 013104 (2020)

CPP 4.6 Mon 11:15 H36

Investigating Twist Angle Dependence of Exciton Resonances in WSe_2/$MoSe_2$ Heterostructures — •Chirag Palekar, Tobias Manthei, Bárbara Rosa, and Stephan Reitzenstein — Institute of Solid State Physics, Technische Universität Berlin, D-10623 Berlin, Germany

Artificially produced TMDC heterostructures (HS) realized by stacking two different TMDC monolayers (ML) are a new class of promising semiconducting heterostructures. Due to their type-II band alignment, TMDC HSs tend to host the spatially indirect interlayer excitons (IX) where electrons and holes are located in conduction and valence bands, respectively, of the different layers. Here we study the twist angle dependence of IX resonances employing micro-photoluminescence excitation (PLE) measurements on twisted WSe_2/$MoSe_2$ heterobilayer. PLE measurements reveal anti-correlation between linewidth and emission energy of IX. Resonant excitation at intralayer exciton energies of constituent ML yields high emission intensity of the IX with linewidth narrowing above 10 meV. We measure a drastic reduction in PL emission from IX for twist angles in the range of 10°- 50° due to large interlayer separation. Moreover, we show a noticeable IX exciton resonance separation which increases as function of twist angle i.e. from 0° (67 meV) to 24° (96 meV) along with observable red shift in IX emission energy. This fundamental study of excitons resonances deepens the current understanding of physics of twisted TMDC heterostructures and paves the way for future experiments and theoretical work.

CPP 4.7 Mon 11:30 H36

Counterintuitive electric-field dependence of weak antilocalization in a bilayer graphene/WSe$_2$ heterostructure — Julia Amann[1], Tobias Völkl[1], Tobias Rockinger[1], Denis Kochan[2], Kenji Watanabe[3], Takashi Taniguchi[3], Jaroslav Fabian[2], Dieter Weiss[1], and •Jonathan Eroms[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Regensburg, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

Heterostructures of bilayer graphene (BLG) and transition metal dichalcogenides (TMDC) were recently proposed as a means of generating a gate-tunable, proximity-induced spin-orbit coupling (SOC) in graphene. Total SOC splitting of the band structure increases monotonically with the out-of-plane electric field, as confirmed by recent charge transport experiments. To elucidate the spin relaxation caused by SOC, weak antilocalization (WAL) experiments are frequently employed. Contrary to the naïve expectation of a monotonic increase of the WAL effect strength with electric field D, we observe a maximum of WAL visibility around $D = 0$. This counterintuitive behaviour originates in the intricate dependence of WAL in graphene on two different spin lifetimes τ_{sym} and τ_{asy}, which are due to spin relaxation caused by the valley-Zeeman and Rashba terms, respectively. Our calculations, based on modeling spin precession by an 8×8 Hamiltonian of BLG with one-sided TMDC show the same non-monotonic dependence on D as the experimental data.

15 min. break

CPP 4.8 Mon 12:00 H36

Millikelvin Spectroscopy on Degenerate Exciton Ensembles in van der Waals Bilayers — •Nihit Saigal[1], Torsten Stiehm[1], Hendrik Lambers[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], Alexander Holleitner[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Walter Schottky Institute and Physics Department, TU Munich, Garching, Germany

Homo- and hetero-bilayers of transition metal dichalcogenides host a rich variety of interlayer exciton (IX) species where the electrons and holes reside in different monolayers. [1] This leads to enhanced lifetimes of IXs and also imparts them with a permanent dipole moment. [1,2] Such IXs provide an ideal platform for exploring many body physics such as dipole-dipole interactions and Bose-Einstein condensation. [2] We have investigated IXs in a heterobilayer of MoSe2 and WSe2 encapsulated in hBN, using temperature, laser power and time dependent photoluminescence (PL) spectroscopy down to millikelvin temperatures. At lowest temperatures and exciton densities, we observe a single low energy peak in the IX PL spectrum which has been attributed to be a signature of degenerate exciton gas. [2] We observe an unexpected nearly excitation power-independent IX energies at lowest temperatures (10 mK to ~10K) that converts into the well-known dipolar blue-shift at elevated temperatures. We acknowledge financial support by DFG via WU 637/4-2 and No. HO 3324/9-2 and SPP2244.

[1] B. Miller et al., Nano Lett. 17, 5229 (2017). [2] L. Sigl et al., Phys. Rev. Research 2, 042044 (R) (2020).

CPP 4.9 Mon 12:15 H36

Infrared photocurrent in transition-metal dichalcogenide heterostructures — Jeong Woo Han[1], Peize Han[2], Yijing Liu[2], Paola Barbara[2], Thomas E. Murphy[3], and •Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Georgetown University, Department of Physics, Washington, 20057 DC, USA — [3]University of Maryland, Institute for Research in Electronics and Applied Physics, College Park, 20740 MD, USA

Heterostructures of transition metal dichalcogenites (TMDCs) have characteristic optical properties like the interlayer excitons due to the band offset between two adjacent TMDC layers. Such heterostructures are promising candidates for photodetectors with higher efficiencies compared to a single TMDC layer, furthermore, the interlayer excitation enables photocurrents at photon energies below the direct bandgap of each of the layers. Here we present measurements on a MoS$_2$/WS$_2$ heterostructure at photon energies of around 800 meV, which is significantly below the interlayer exciton. The cross-shaped structure of our samples allows measurements of the heterostructure as well as each individual layer. While at high photon energies photocurrents are observed in each of the layers, the low photon energy only leads to a photocurrent when the heterostructure is illuminated. We interpret this effect to be caused by intraband absorption and subsequent interlayer tunneling.

CPP 4.10 Mon 12:30 H36

Strong exciton-plasmon coupling in hybrids of 2D semiconductors and metal supercrystals — •Lara Greten, Robert Salzwedel, Malte Selig, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of transition metal dichalcogenides (TMDC) are direct semiconductors that exhibit tightly bound excitons with uniquely large optical amplitudes. Thus, they are promising for optoelectronic applications and a prime example to investigate excitonic effects.

Complementary, plasmonic supercrystals, that are arrays of metal nanoparticles, support collective plasmon modes. They facilitate an impressive amplification of the electric near-field which allows to tailor electric fields on the nano-scale.

In the presented work, we theoretically consider exciton-plasmon coupling in a hybrid structure of a TMDC layer interacting with a single metal nano-particle or a two-dimensional supercrystal. For this purpose, we develop a Maxwell-Bloch theory where the excitons are described within the Heisenberg equation of motion framework and the metal nano-particles are treated as coupled dipoles in Mie theory.

Our studies reveal new "plexcitonic" eigenstates of the hybrid system. Furthermore, we are able to compute the scattered light in the near- and far-field explicitly and identify signatures of strong exciton-plasmon coupling featuring a Rabi splitting of tens of meV.

CPP 5: Wetting, Droplets and Microfluidics (joint session DY/CPP)

Time: Monday 10:00–12:15 Location: H19

CPP 5.1 Mon 10:00 H19

Lattice Boltzmann simulations of dense suspensions of soft particles with interface viscosity — •Fabio Guglietta[1], Othmane Aouane[1], Francesca Pelusi[1], Marcello Sega[1], and Jens Harting[1,2] — [1]Helmholtz Institute Erlangen-Nürnberg, Germany — [2]Department of Chemical and Biological Engineering and Department of Physics, FAU Erlangen-Nüremberg, Germany

Interface viscosity (IV) plays a major role in the dynamics of single droplets and viscoelastic capsules by influencing their transient dynamics and steady-state deformation. For example, it has recently become clear that numerical models for red blood cells must include IV to account for their realistic description. Therefore, IV can be expected to play a significant role in determining also the dynamics and rheology of their dense suspensions. However, as no detailed investigation exists on the effects of IV in the dense suspensions of soft capsules, we aim to fill this gap by including it in computational fluid dynamics models. Here, we address this problem for the first time by performing numerical simulations in the framework of the immersed boundary - lattice Boltzmann method. This approach proved to be a valid numerical tool to provide a realistic description of soft particles immersed in Newtonian fluids. We employ a recent numerical model to account for IV by relying on the discretised Boussinesq-Scriven tensor, which provides a continuum description of a 2D viscous fluid. We show that the IV influences (a) the time it takes for particles to deform during the transient phase and (b) the final shape of the particles in the steady-state at different volume fraction values.

CPP 5.2 Mon 10:15 H19

Wetting dynamics of droplets: an immersed boundary lattice Boltzmann approach — •Francesca Pelusi[1], Othmane Aouane[1], Fabio Guglietta[1], Marcello Sega[1], and Jens Harting[1,2] — [1]Helmholtz Institute Erlangen-Nürnberg, Germany — [2]Department of Chemical and Biological Engineering and Department of Physics, FAU, Germany

Many applications in computational fluid dynamics require the immersed boundary (IB) method to couple the dynamics of well-defined structures with that of a surrounding fluid. If the latter is simulated with a lattice Boltzmann (LB) method, the resulting IBLB approach is known to be a very versatile tool, for example, in studying dense suspensions of red blood cells. However, little attention has been devoted so far to applying this approach to substrate wetting problems. Here, we report on an IBLB-based investigation of the wetting of droplets interacting with a solid surface. In our model, the droplet surface tension contributes to the force the droplet (structure) communicates to the surrounding fluid. We characterize Newtonian droplets' static and dynamic contact angles and show how surface/IB-nodes interaction tuning allows obtaining the desired wetting properties. Furthermore, the flexibility of the IBLB approach will enable us to model non-Newtonian surface rheology, opening the possibility of simulating the unusual wetting behavior of gallium droplets. Indeed, liquid gallium develops an oxide layer at the liquid surface when in contact with the oxygen, which affects its adhesive properties with significant consequences for its high-tech applications, such as catalysis.

CPP 5.3 Mon 10:30 H19

Viscosity-induced Destabilization of a Liquid Sheet in Inertial Microfluidics — •Kuntal Patel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Lab-on-a-chip devices based on inertial microfluidics function between Stokes and turbulent regimes, which enables to achieve high throughput. In the present work, we study the motion of a liquid sheet of thickness t_s and viscosity μ_1 in a two-dimensional microchannel of width w, filled with a viscous fluid (viscosity μ_2, $m = \mu_2/\mu_1 > 1$). At finite Reynolds number Re, a small perturbation at the interfaces separating the sheet from the surrounding fluid can result in a rapid destabilization of interfaces and may lead to a break-up. The present work gives a proof-of-concept of how viscosity-driven interfacial instability can be exploited for a controlled droplet production in inertial microfluidics. Such microfluidic droplets are utilized in food and pharmaceutical related applications and as chemical reactors in Lab-on-a-chip devices.

In our computational linear stability analysis based on the Orr-Sommerfeld equation, we observe that the growth rate of the fastest growing mode ξ^* increases with Re. Furthermore, the dependence of ξ^* on m and t_s is quantified by the scaling law $\xi^* \propto m t_s^{2.5}$, which is valid for thin sheets in moderate Re flows with relatively weak interfacial tension Γ. In the second part, our lattice Boltzmann simulations starting from a single-mode perturbation of wavelength λ reveal that the interfacial instability causes the liquid sheet to break up and ultimately to form droplets when $\lambda \geq 0.5w$. We also identify different interface breakup mechanisms leading to droplet formation.

CPP 5.4 Mon 10:45 H19

Imaging, Analysis and Sorting in Microfluidic Systems: Correlative Multi-Contrast, Multi-Parameter Applications — •Tobias Neckernuss[1], Patricia Schwilling[2], Jonas Pfeil[1,2], Daniel Geiger[1], and Othmar Marti[2] — [1]Sensific GmbH — [2]Institute for Experimental Physics, Ulm Univeristy

Droplet-based microfluidics is a promising approach in biology, pharmacy, medicine, and lab-on-a-chip applications. One remaining problem is the lack of a suitable fast image-based detection method that enables droplet- and content-based analysis and sorting with rates fast enough to be sufficient for high-throughput measurements and to enable surveilled lab scale production. We demonstrate recent advances for high-speed, real-time, image-based analysis and manipulation of microfluidic systems. With rates of up to 3000 particles or droplets per second we show applications of our system in the field of droplet-based microfluidics. Here, we concentrate on droplet-content analysis and have a sneak look at further potential applications in biology and image-based cell analysis. We introduce new contrast types for image-based analysis like brightfield, darkfield, phase contrast, fluorescence and combinations thereof. Combining new cutting edge hardware technology with specifically tailored software and integration of external lab infrastructure enables us reach new dimensions in image based particle analysis and sorting.

15 min. break

CPP 5.5 Mon 11:15 H19

the obstacle effect on soft sphere discharging in quasi-2D silo — •Jing Wang[1], Kirsten Harth[1,2], Dmitry Puzyrev[1], and Ralf Stannarius[1] — [1]Institute of Physics, Otto von Guericke University Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]Department of Engineering, Brandenburg University of Applied Sciences, Magdeburger Straße 50, D-14770 Brandenburg an der Havel, Germany

Soft smooth particles in silo discharge show their own characteristics, for example, non-permanent clogging and intermittent flow. We conduct experiment on soft, low-frictional hydrogel spheres compred with hard, frictional spheres in a quasi-2D silo. We introduce a competitive behavior of these spheres during their discharge by placing an obstacle in front of the outlet of the silo. High-speed optical imaging is applied to capture the process of discharge. By the method of particle tracking velocimetry (PTV), the fields of velocity, egress time, packing fraction, and kinetic stress are analysed in the study.

CPP 5.6 Mon 11:30 H19

Coalescence of isotropic and nematic droplets in quasi 2D liquid crystal films — •Christoph Klopp, Alexey Eremin, and Ralf Stannarius — Institute for Physics, Otto von Guericke University Magdeburg, Germany

Coalescence of droplets is ubiquitous in nature and modern technology. Various experimental and theoretical studies explored droplet dynamics in three dimensions (3D) and on two-dimensional (2D) solid or liquid substrates, e.g. [1-3]. Here, we demonstrate coalescence of isotropic and nematic droplets in quasi-2D liquids, viz. overheated smectic A freely suspended films. We investigated their dynamics experimentally and measured the shape deformation during the entire merging process using high-speed imaging and interferometry. This system is a unique example where the lubrication approximation can be directly applied, and the smectic membrane plays the role of a precursor film. Our studies reveal the scaling laws of the coalescence time depending on the droplet size and the material parameters. We also compared the dynamics of isotropic and nematic droplets and additionally analyzed the results based on an existing model for liquid lens coalescence on liquid and solid surfaces [4].

Acknowledgements: This study was supported by DLR and DFG within the OASIS and OASIS-Co projects WM2054 and STA 425/40.

References: [1] J. D. Paulsen et al., Nat. Commun., 5, 3182 (2014) [2] D. G. A. L. Aarts et al., Phys. Rev. Lett., 95, 164503 (2005). [3] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [4] C. Klopp et al., Langmuir, 36, 10615 (2020)

CPP 5.7 Mon 11:45 H19

Using feedback-controlled thermoviscous flows to precisely position microparticles — •Elena Erben, Antonio Minopoli, Nicola Maghelli, Benjamin Seelbinder, Iliya D. Stoev, Sergei Klykov, and Moritz Kreysing — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Optical positioning of microscale objects has proven key for advancing fundamental biological research and holds great potential for other disciplines as well. The most widely used among these methods are optical tweezers which enable the precise control and manipulation of multiple particles. However, they require probes of high refractive index contrast and low absorption and exclude the use of photosensitive samples. Here we present a novel optofluidic technique that leverages optical-control capabilities and the gentle nature of hydrodynamic flows, thus lifting the aforementioned constraints. Our approach is based on optically-induced thermoviscous flows generated by the repeated scanning of a moderately heating infrared laser beam [1]. We have combined thermoviscous flows with feedback control to confine micron-sized particles with a precision of up to 24 nm without exposing them directly to laser light [2]. Recently, we extended this approach beyond single-object manipulation to further enable simultaneous control of multiple particles. With this contribution, we furthermore discuss combinations with implicit force sensing [3] and the potential for future application in and beyond the life science sector.

[1] Weinert et al., *Phys. Rev. Lett.*, 2008; [2] Erben et al., *Opt. Express*, 2021; [3] Stoev et al., *eLight*, 2021.

CPP 5.8 Mon 12:00 H19

Active thin films — •Tilman Richter[1], Paolo Malgaretti[1], Stefan Zitz[2], and Jens Harting[1] — [1]Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen- Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany — [2]Roskilde University, Department of Science and Environment, Roskilde, Denmark

Thin liquid films are important for many microfluidic applications such as printing or coating of e.g. printable electronics or photovoltaic cells where a evenly spread thin film of certain properties is of utmost importance. It is well known that a thin film on a solid substrate can be unstable and droplet formation may arise, especially for very thin films. The dynamics of thin liquid films and their instability has been the subject of intensive experimental, analytical, and numerical studies, the latter often based on the thin film equation. We propose a set of newly developed equations for the influence of chemical active colloids suspended in a thin liquid film based on the lubrication approximation, advection-diffusion and, the Fick-Jackobs approximation. For this novel set of equations we perform a linear stability analysis (LSA) that reveals surprisingly interesting dynamics. We identify the subset of parameters for which the thin film becomes stable, as well as a variety of different dominating wave-modes. This allows us to control not only the stability but also the droplet size distribution after film rupture. In order to assess the asymptotic state of the thin film, the LSA results are compared against numerical simulations using the Lattice Boltzmann method.

CPP 6: Active Matter 1 (joint session BP/CPP/DY)

Time: Monday 10:30–12:45 Location: H16

Invited Talk CPP 6.1 Mon 10:30 H16

Computer simulations of self-motile active droplets and colloid-active gels composites — •Davide Davide Marenduzzo — School of Physics and Astronomy, University of Edinburgh, Edinburgh, UK

In this talk we will show results from computer simulations probing the behaviour of composite materials based on active gels.

In the first part of the talk we will investigate the behavior of active nematic or cholesteric droplets inside an isotropic fluid. In different regions of parameter space, we find regular motility and chaotic behaviour, and discuss the relevance of these results to biophysical systems such as microbial motility.

In the second part of the talk, we will study the dynamics of a dispersion of passive colloidal particles in an active nematic host. We find that activity induces a dynamic clustering of colloids even in the absence of any preferential anchoring of the active nematic director at the particle surface. When such an anchoring is present, active stresses instead compete with elastic forces and re-disperse the aggregates observed in passive colloid-liquid crystal composites.

CPP 6.2 Mon 11:00 H16

Chloroplasts in dark-adapted plants show active glassy behavior — •Nico Schramma, Cintia Perugachi Israëls, and Mazi Jalaal — University of Amsterdam, Amsterdam, Netherlands

Photosynthesis in plants is one of the main drivers for the survival of whole ecosystems on earth. To guarantee the efficiency of this process, plants have to actively adapt to ever-changing light conditions. On large time scales plants can grow towards the light. However, this process is too slow to adapt towards transient stimuli. To do this plants can re-arrange the intracellular structure by the active motion of chloroplasts on short timescales. These organelles are confined between the cell membrane and vacuole and can move inside the cytoplasm via actin polymerization forces. Remarkably, the simple - yet elegant - interplay of light-sensing and active forces leads to various modes of collective motion. Here, we show that the chloroplasts under dark conditions are densely packed systems, driven by a-thermal noise and can exhibit active glassy motion. Furthermore, we aim to establish chloroplast motion as a new framework to study the dynamics of light-controlled dense biological systems featuring intriguing dynamic phase transitions.

CPP 6.3 Mon 11:15 H16

Activity-induced polar patterns of filaments gliding on a sphere — •Chiao-Peng Hsu, Alfredo Sciortino, Yu Alice de la Trobe, and Andreas Bausch — Center for Protein Assemblies and Lehrstuhl für Zellbiophysik E27, Physics Department, Technische Universität München, Garching, Germany

Active matter systems feature the ability to form collective patterns as observed in a plethora of living systems, from schools of fish to swimming bacteria. While many of these systems move in a wide, three-dimensional environment, several biological systems are confined by a curved topology. The role played by a non-Euclidean geometry on the self-organization of active systems is not yet fully understood, and few experimental systems are available to study it. Here, we introduce an experimental setup in which actin filaments glide on the inner surface of a spherical lipid vesicle, thus embedding them in a curved geometry. We show that filaments self-assemble into polar, elongated structures and that, when these match the size of the spherical geometry, both confinement and topological constraints become relevant for the emergent patterns, leading to the formation of polar vortices and jammed states. These results experimentally demonstrate that activity-induced complex patterns can be shaped by spherical confinement and topology.

15 min. break

CPP 6.4 Mon 11:45 H16

The effect of chiral flows on pattern formation on active cell surfaces — Lucas Wittwer[2], Eloy de Kinkelder[1], and •Sebastian Aland[1,2] — [1]TU Freiberg — [2]HTW Dresden

Mechanochemical processes play a crucial role during morphogenesis, the formation of complex shapes and tissues out of a single cell. On the cellular level, the actomyosin cortex governs shape and shape changes. This thin layer of active material underneath the cell surface exerts an active contractile tension, the strength of which being controlled by the concentration of force-generating molecules. Advective transport of such molecules leads to a complex interplay of hydrodynamics and molecule concentration which gives rise to pattern formation and self-organized shape dynamics. In this talk, we present a novel numerical model to simulate an active viscoelastic surface immersed in viscous fluids. The resulting patterning, flows and cell shape dynamics are shown for different parameter configurations. It is further demonstrated that adding a chiral (i.e. counter-rotating) force at the cell surface can promote a ring of high molecule concentration and facilitate cell division.

CPP 6.5 Mon 12:00 H16

Premelting controlled active matter in ice — •Jeremy Vachier[1] and John S. Wettlaufer[1,2] — [1]Nordita, KTH Royal Institute of Technology and Stockholm University, Hannes Alfvéns väg 12, SE-106 91 Stockholm, Sweden — [2]Yale University, New Haven, Connecticut 06520-8109, USA

Self-propelled particles can undergo complex dynamics due to a range of bulk and surface interactions. In the case of a foreign particle inside a subfreezing solid, such as a particle in ice, a premelted film can form around it allowing the particle to migrate under the influence of an external temperature gradient, which is a phenomenon called thermal regelation. It has recently been shown that the migration of particles of a biological origin can accelerate melting in a column of ice and thereby migrate faster. We have previously shown that the effect of regelation plays a major role in the migration of inert particles and impurities inside ice, with important environmental implications. In particular, the question of how the activity affects a particle's position over time is essential for paleoclimate dating methods in ice cores. We re-cast this class of regelation phenomena in the stochastic framework of active Ornstein-Uhlenbeck dynamics and make predictions relevant to this and related problems of interest in geophysical and biological problems.

CPP 6.6 Mon 12:15 H16

Emergent collective behavior of active Brownian particles with visual perception — •Rajendra Singh Negi, Roland G.

Winker, and Gerhard Gompper — Theoretical Physics of Living Matter, Institute of Biological Information Processing (IBI-5), Forschungszentrum Jülich, 52425 Jülich, Germany

Collective behavior of self-propelled agents emerges from the dynamic response of individuals to various input signals [1,2]. One such input signal is visual perception. We explore the behavior of a model of self-steering active Brownian particles with visual perception in two dimensions [3]. Several non-equilibrium structures like motile worms, worm-aggregate coexistence, aggregates, and a dilute-gas phase are obtained, depending on the system parameters. The strength of the response to the visual signal, vision angle, packing fraction,rotational diffusion, and activity (velocity v_0) determine the location and extent of these phases in the phase diagram. The radius-of-gyration tensor is used to distinguish between the worm and the aggregate phase. Our results help to understand the collective behavior of cognitive self-propelled particles, like animal herds and micro-robotic swarms.

[1]. J. Elgeti, R. G. Winkler, and G. Gompper, Rep. Prog. Phys. **78**, 056601 (2015).

[2]. M. R. Shaebani, A. Wysocki, R. G. Winkler, G. Gompper, and H. Rieger, Nat. Rev. Phys. **2**, 181 (2020).

[3]. L. Barberis and F. Peruani, Phys. Rev. Lett. **117**, 248001 (2016).

CPP 6.7 Mon 12:30 H16

Diffusiophoretic propulsion of an isotropic active particle near a finite-sized disk — •Abdallah Daddi-Moussa-Ider[1], Andrej Vilfan[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Göttingen, Germany — [2]Jozef Stefan Institute, 1000 Ljubljana, Slovenia — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We employ a far-field analytical model to quantify the leading-order contribution to the induced phoretic velocity of an isotropic active colloid near a finite-sized disk of circular shape resting on an interface separating two immiscible viscous incompressible Newtonian fluids. To this aim, we formulate the solution of the phoretic problem as a mixed-boundary-value problem which we then transform into a system of dual integral equations on the inner and outer domains. Depending on the ratio of different involved viscosities and solute solubilities, the sign of phoretic mobility and chemical activity, as well as the ratio of particle-interface distance to the radius of the disk, we find the isotropic active particle to be repelled from the interface, be attracted to it, or reach a stable hovering state and remain immobile near the interface. Our results may prove useful in controlling and guiding the motion of self-propelled phoretic active particles near aqueous interfaces.

Reference: A. Daddi-Moussa-Ider, A. Vilfan, and R. Golestanian, *J. Fluid Mech.* **940** A12 (2022)

CPP 7: Wetting, Fluidics and Liquids at Interfaces and Surfaces

Time: Monday 10:45–13:00 Location: H39

CPP 7.1 Mon 10:45 H39

Coupling of liquid-liquid phase separation and wetting dynamics — •Youchuang Chao, Olinka Ramírez-Soto, Christian Bahr, and Stefan Karpitschka — Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

The interplay of phase separation and surface wetting is of great interest for various fields, ranging from industrial applications of oil recovery to the formation of membraneless organelles in living cells. Most of previous studies focus on understanding the interaction of phase separation with static wetting, i.e., pinned contact line conditions; nevertheless, how phase separation interacts with dynamical wetting, for instance, advancing contact lines is still unclear. Here, using highly mobile, Marangoni-contracted droplets of evaporating, binary liquid mixtures with a well-defined miscibility gap on fully wetting substrates, we explore the interplay of phase separation and wetting dynamics. Interestingly, we observe an abrupt wetting transition: from a contracted droplet state in the one-phase region to an actively driven spreading motion in the two-phase region; This is caused by the strong coupling of liquid-liquid phase separation and advancing contact lines, together with effects of evaporative enrichment and surface forces. Our finding may enable the development of novel surface processing strategies.

CPP 7.2 Mon 11:00 H39

Liquid phase separation during soft dynamic wetting — •Lukas Hauer[1], Zhuoyun Cai[2], Jonathan T. Pham[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Chemical and Materials Engineering, University of Kentucky,Lexington, Kentucky, USA

Droplets sitting on soft substrates deform the material around the three-phase contact line, i.e., the formation of the wetting ridge. While on liquid films the ridge geometry is solely governed by capillarity, on (visco)elastic films elastic contributions add to the ridge geometry. Recently, on (visco)elastic materials a capillary induced phase-separated region of pure liquid was observed. Here, we investigate this phase separation on crosslinked PDMS films with differing amounts of free oligomer chains during dynamic wetting. We let droplets forcefully slide over PDMS films while monitoring the ridge zone with laser scanning confocal microscopy. Different dyes in the crosslinked network and in the free oligomers enable discrimination between the two phases. We find that phase-separation competes with the motion of the droplet: by tuning the droplets' speed, the phase-separated ridge height ranges from > 30 μm (at 5 μm/s) to no phase separation at all for fast speeds.

15 min. break

CPP 7.3 Mon 11:30 H39

Deep learning to analyze sliding drops — •Sajjad Shumaly, Fahimeh Darvish, Xiaomei Li, Alexander Saal, Chirag Hinduja, Werner Steffen, Oleksandra Kukharenko, Rüdiger Berger, and Hans-Jürgen Butt — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany

Investigation of drop sliding forces requires knowledge of the shape of the drop close to the three-phase contact line. State-of-the-art contact angle measurement methods are designed for analyzing symmetric and high-resolution images of the drop. The analysis of videos of drops sliding down a tilted plane is hampered due to the low-resolution of the cutout area where the drop is visible. The drop is just a part of the whole image. In addition, drops sliding down a tilted plate are unsymmetrical in shape and the three-phase contact line may deform due to the sticky points.

In order to increase the accuracy of the measured contact angle, we trained a deep learning-based super-resolution model with an up-scale ratio of 3, i.e. the trained model is able to enlarge droplet images 9 times. In the second step, we performed an optimized polynomial fitting approach to measure the contact angle even for symmetric, asymmetric, or deformed droplets without the need for liquid parameters. To find the best parameters for polynomial fitting in our special problem, we conducted a systematic experiment using synthetic images.

CPP 7.4 Mon 11:45 H39

How often a Drops Sticks and Slips at a Wetting Transition — Chirag Hinduja[1], Alexandre Laroche[1,2], Sajjad Shumaly[1], Yujiao Wang[3,4], Doris Vollmer[1], Hans-Jürgen Butt[1], and •Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]University of Zurich, 8057 Zurich, Switzerland — [3]Key Laboratory of Interfacial Physics and Technology, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201800, China — [4]University of Chinese Academy of Sciences, Beijing 100049, China

We will discuss forces of sliding drops at a sharp wetting transitions featuring no topographic variation. Such surfaces with different wetting properties were made from chemical vapor deposition of trichlorooctylsilane (OTS) and tri-chloro(perfluoro) octylsilane (PFOCTS). We observed that drops sliding from an area of low to high contact angle hysteresis exhibit two force maxima. The drop motion is characterized by pinning of the advancing and receding contact lines, respectively. Accordingly, the motion of the drop follows two stick-slip processes.

Drops sliding from an area of high to low contact angle hysteresis exhibit a single local force maximum, a single stick process, but two slip processes.

Sliding forces of drops were measured by a novel tool named scanning Drop Adhesion Force Instrument (sDAFI) which we use to image, locate and characterize wetting properties of cm-large areas with a resolution down to the micrometer-scale.

CPP 7.5 Mon 12:00 H39

Tunable lamellar topography driven by wetting dynamics — •Gissela Constante[1], Indra Apsite[1], Paul Auerbach[2], Sebastian Aland[2], Dennis Schönfeld[3], Thorsten Pretsch[3], Pavel Milkin[1], and Leonid Ionov[1,4] — [1]University of Bayreuth, Bayreuth, Germany — [2]Hochschule für Technik und Wirtschaft Dresden, Dresden, Germany — [3]Fraunhofer Institute for Applied Polymer Research IAP, Postdam, Germany — [4]Bavarian Polymer Institute, Bayreuth, Germany

The fabrication of switchable surfaces has been of interest in several fields such as biotechnology, industry, and others. The selection of materials and methods is crucial to provide proper control on the tunable surface. In this research, an exceptional high aspect ratio lamellar surface topography was fabricated by melt-electrowriting of microfibers of a shape-memory thermo-responsive polyurethane. Two different types of stimuli: temperature and light exposition were applied to modify the mechanical properties of shape memory polymer and thus program deformation and recovery of the surface. Wetting studies showed that the deformation of the high aspect ratio lamellar surface can be tunned not only manually, but as well by a liquid droplet. This behavior is controlled by temperature changes during direct heating/cooling or by exposure to light. The liquid in combination with thermo-responsive topography presents a new type of wetting behavior. This feature opens the possibility to apply such topographies for the design of smart elements for microfluidic devices, for example, smart valves.

CPP 7.6 Mon 12:15 H39

Gradient dynamics model for sessile drop evaporation in a gap: from simple to applied scenarios — •Simon Hartmann[1], Uwe Thiele[1], Christian Diddens[2], and Maziyar Jalaal[3] — [1]Institut für Theoretische Physik and Center for Nonlinear Science, Universität Münster — [2]Physics of Fluids group, Max Planck Center Twente for Complex Fluid Dynamics, and J. M. Burgers Center for Fluid Dynamics, University of Twente — [3]Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam

We consider an evaporating drop of volatile partially wetting liquid on a rigid solid substrate. In addition, the setup is covered with a plate, forming a narrow gap with the substrate. First, we develop an efficient mesoscopic description of the liquid and vapor dynamics in a gradient dynamics form. It couples the diffusive dynamics of the vertically averaged vapour density in the narrow gap to an evolution equation for the drop profile. The dynamics is purely driven by a free energy functional that incorporates wetting, bulk and interface energies of the liquid as well as vapour entropy.

Subsequently, we employ numerical simulations to validate the model against both experiments and simulations based on Stokes equation. Finally, we show that the gradient dynamics approach allows for extensions of our model to cover more intricate scenarios, e.g., spreading drops of volatile liquid on polymer brushes or on porous media.

CPP 7.7 Mon 12:30 H39

Dewetting of thin lubricating films under aqueous drops on high and low surface energy surfaces — •Bidisha Bhatt, Shivam Gupta, Vasudevan Sumathi, Sivasurender Chandran, and Krishnacharya Khare — Indian Institute of Technology Kanpur, Kanpur, India

Understanding the stability of thin liquid films under different environments is important due to their potential applications, such as coatings, paints, and printing, to name a few. In this work, we investigate the stability of thin liquid films of a lubricating fluid under aqueous drops on slippery surfaces. Lubricating films under aqueous drops are found stable when the total excess free energy of the system is positive, which otherwise would dewet into droplets on hydrophilic surfaces. The dewetting dynamics and the apparent contact angle of the aqueous drop depend on the thickness of the lubricating film and the final morphology depends on interfacial boundary conditions between film and the substrate. However, the lubricating films on hydrophobic surfaces are stable under the aqueous drops, yet they can be destabilized using external perturbations like an electric field. Due to the electric field, surface capillary waves are generated at the film-drop interface, and the amplitude of the waves grows exponentially with time, similar to spinodal dewetting. Experimentally observed wavelength and growth rate of the surface capillary waves show good agreement with the theoretically predicted value using linear stability analysis. The dewetted droplets coalesce and form a uniform film again upon removing the applied voltage, making the dewetting process fully reversible.

CPP 7.8 Mon 12:45 H39

Cloaking Transition of Droplets on Lubricated Brushes — •Rodrique Badr[1], Friederike Schmid[1], Doris Vollmer[2], and Lukas Hauer[2] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Max Plank Institute for Polymer Physics, Mainz, Germany

We study the equilibrium properties and wetting behavior of a simple liquid on a polymer brush, with and without the presence of lubricant. We investigate the behavior of the brush in terms of grafting density and the amount of lubricant present. As for the wetting behavior, we study a sessile droplet on top of the brush. Our model and choice of parameters results in the formation of a wetting ridge and in the cloaking of the droplet by the lubricant, a phenomenon that is observed experimentally and is of integral importance to the dynamics of sliding droplets. We quantify the cloaking in terms of its thickness, which increases with the amount of lubricant present, and provide thermodynamic theory to explain the behavior. In addition, we investigate the dependence of contact angles on the size of the droplet and the possible effect of line tension, as well as the dependence on the cloaking/lubrication of the brush.

CPP 8: Focus Session: Photonic Structures from Polymer and Colloidal Self-Assembly

organized by Ilja Gunkel (University of Fribourg) and Bodo Wilts (University of Salzburg)

Time: Monday 15:00–17:15 Location: H38

Invited Talk CPP 8.1 Mon 15:00 H38

Stimuli-Responsive Opal Films based on Core-Shell Particle Self-Assembly — •Markus Gallei — Lehrstuhl für Polymerchemie, Universität des Saarlandes, Campus C4 2, Saarbrücken

In the last decade stimuli-responsive polymers have proven their feasibility for a wide range of important applications. These polymers are capable of changing their conformation, solubility, or they can even break or form covalent bonds upon a change of temperature or pH, light irradiation or by electrochemical stimuli, or combinations thereof. The presentation will focus on materials, which contain at least one selectively addressable segment, either chemically or physically. Functional porous nanostructures based on inverse opal films obtained after shear-induced particle self-assembly will be highlighted and discussed in more detail. In the case of soft colloidal crystal and their inverted structures, external triggers additionally lead to a remarkably fast and reversible change of their intriguing optical properties. Moreover, such opal structures can be used for the design of smart catch and release systems based on responsive moieties, but also as soft templates for ceramic materials. The talk will give some recent examples for the rational design of functional organic as well as hybrid porous materials with hierarchical architectures. Some of the highlighted polymer or polymer-templated structures can be advantageously used for direct conversion into ordered ceramic or carbonaceous materials. Herein presented preparation strategies will pave the way for a manifold of applications in the field of sensing and robust membrane technologies.

CPP 8.2 Mon 15:30 H38

Strategies for increased colour saturation in colloidal photonic crystals — •Gudrun Bleyer[1], Carina Bittner[1], Lukas Roemling[1], Nico Nees[2], Eric Goerlitzer[1], and Nicolas Vogel[1] — [1]Institute of Particle Technology (LFG), FAU, Erlangen, Germany

— [2]Chair of Applied Mathematics, FAU, Erlangen, Germany

Monodisperse polystyrene nanoparticles are easily synthesized using surfactant free emulsion polymerization, making them ideal accessible building block for photonic crystals via self-assembly.

However, structures made only with polystyrene display a whitish hue of colour as incoherent scattering at defects in the crystal structure overlaps with the photonic stop band from constructive interference. We investigate how the colour saturation in colloidal photonic crystals depends on the local and global ordering of the particles and the absorptive properties of additive materials.

First, we assemble photonic crystals using two methods resulting in structures displaying different defect characteristics. We then correlate the photonic properties as a function of these defects using correlative microscopy connecting optical imaging, reflectance spectra and SEM measurements to establish the structure-property relationship.

Secondly, we introduce absorbing material at defined positions within the colloidal photonic crystal with the goal to optimize not only the amount but the absorber position as well, allowing for an optimized colour saturation.

Invited Talk CPP 8.3 Mon 15:45 H38

Self-assembled photonic pigments from bottlebrush block copolymers — •Richard Parker, Tianheng Zhao, Zhen Wang, Clement Chan, and Silvia Vignolini — Yusuf Hamied Department of Chemistry, University of Cambridge, United Kingdom

The self-assembly of bottlebrush block copolymers (BBCPs) into photonic materials has drawn significant attention due to the flexibility and diversity of the building blocks that can be synthesised. In this talk we will introduce a robust strategy for the fabrication of hierarchical photonic pigments via the confined self-assembly of BBCPs within emulsified microdroplets. By utilising an amphiphilic BBCP and optimising the emulsification conditions, we will demonstrate the formation of structurally coloured particles with a correlated disordered structure (i.e. a photonic glass) and compare them to particles with a highly-ordered concentric lamellar structure (i.e. a 1D photonic crystal). The mechanisms behind these two different architectures will be proposed and methods to tune the reflected colour of the respective systems considered. Finally, the strengths and weaknesses of the two approaches will be summarised in terms of the optical properties of the particles, the scalability of the approach and their viability as real-world colorants.

CPP 8.4 Mon 16:15 H38

Elucidating the chiral self-assembly of cellulose nanocrystals for photonic films — •Thomas Parton, Richard Parker, Gea van de Kerkhof, Aurimas Narkevicius, Johannes Haataja, Bruno Frka-Petesic, and Silvia Vignolini — Department of Chemistry, University of Cambridge, United Kingdom

Cellulose nanocrystals (CNCs) are naturally-sourced elongated nanoparticles that form a cholesteric colloidal liquid crystal phase in suspension. Interestingly, this helicoidal arrangement can be preserved upon drying to create films with vibrant structural colour. However, while CNCs have drawn significant attention as a way to produce sustainable photonic materials, the underlying mechanism by which chirality arises in the mesophase remains unclear. Although the morphology of individual CNCs is believed to play an important role, most particles are not strongly twisted, and the suspensions exhibit considerable polydispersity in both particle size and shape.

In this study, we performed an in-depth morphological analysis of CNCs observed using transmission electron microscopy (TEM) and atomic force microscopy (AFM). We sequentially tuned the size and shape of the CNCs using ultrasonication and correlated the morphology of individual nanoparticles with their ensemble liquid crystalline behaviour and photonic response. This analysis revealed that a subpopulation of CNC “bundles” (i.e. clusters of laterally-bound elementary crystallites) act as chiral dopants, analogous to those used for molecular liquid crystals, and are therefore essential for the formation of the cholesteric phase.

15 min. break

Invited Talk CPP 8.5 Mon 16:45 H38

Hierarchically structured mechanochromic deformation-sensing pigments — •Jessica Clough[1], Cédric Kilchoer[1], Bodo Wilts[1,2], and Chris Weder[1] — [1]Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, Fribourg 1700, Switzerland — [2]Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Str. 2a, 5020 Salzburg, Austria.

Mechanochromic materials can change their colour in response to mechanical force and are useful for fundamental studies as well as practical applications. A versatile platform with extended sensing capabilities would be valuable for monitoring complex mechanical behaviours and failure events. Here, we report that this is possible by combining photonic structures, which alter their reflection upon deformation, and covalent mechanophores, whose absorption changes upon mechanically induced bond scission, in hierarchically structured assemblies. This was achieved by synthesising microspheres of an elastic polymer with spiropyran-based cross-links and incorporating non-close-packed silica nanoparticles into this matrix. The shift of the reflection band produced by the silica is noticeable at less than 1% strain, while the conversion of the spiropyran can require strains exceeding 50%. The two responses can be tailored via the silica content and the cross-link density. The mechano-sensing pigments can readily be incorporated into different materials of interest and probe local deformations from within. This was demonstrated by monitoring high-strain deformation of poly(dimethyl siloxane) in compression and local strain field variations caused by the necking of semicrystalline polyethylene.

CPP 9: Modeling and Simulation of Soft Matter (joint session CPP/DY)

Time: Monday 15:00–17:45 Location: H39

CPP 9.1 Mon 15:00 H39

Machine Learning of consistent thermodynamic models using automatic differentiation — •David Rosenberger[1], Kipton Barros[2], Timothy Germann[2], and Nicholas Lubbers[2] — [1]Freie Universität Berlin, Berlin, Germany — [2]Los Alamos National Laboratory, Los Alamaos, NM, USA

Instead of fitting suitable analytical expressions to thermophysical data, we propose to combine automatic differentiation and artificial neural networks (ANNs) to obtain complex equations of state (EOS) for arbitrary systems. Rather than training directly on the properties of interest, we train an ANN on a model free energy whose partial derivatives match the thermophysical properties measured in experiment. We show that this method is advantageous over direct learning of thermodynamic properties, in terms of both accuracy and the exact preservation of the Maxwell relations. Furthermore, the method can implicitly solve the integration problem of computing the free energy of a system without explicit integration given appropriate data to learn from.

CPP 9.2 Mon 15:15 H39

Atomistic Machine Learning for Aqueous Ionic Solutions — •Philip Loche, Kevin K. Huguenin-Dumittan, and Michele Ceriotti — Laboratory of Computational Science and Modeling, IMX, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Accurate modeling of matter at the atomic scale requires to simultaneously account for the quantum nature of the chemical bond - that usually manifests itself on short time and length scales - and long-range interactions, such as electrostatics and dispersion, that occur on a large scale and often result in phenomena with a long characteristic time. Electronic structure calculations provide an accurate description of both quantum and long-range effects, but are computationally demanding, and scale poorly with system size. Machine learning (ML) approaches have emerged as a very effective strategy to build surrogate models that provide comparable accuracy at a fraction of the cost, but the most widespread techniques base their efficiency and transferability on a local description of atomic structure, which makes them ill-equipped to deal with long-range effects.

Here, we are going to to connect local and long range physics in a data driven ML approach by applying the current ML techniques to, condensed-phase systems, involving the characterization of aqueous ionic solutions. We show that only a combination of a long and a short range approach is able to predict short distanced molecular vibrations as well a long ranged ionic screening lengths.

CPP 9.3 Mon 15:30 H39

Identification of glass transition temperature for polymer melts using data-driven methods — •Atreyee Banerjee, Hsiao-ping Hsu, Oleksandra Kukharenko, and Kurt Kremer — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

On fast cooling, the dynamics of polymer melts slow down exponentially, leading to solid glassy states without any drastic change in the structural structure. We employ data-driven methods based on purely confomational fluctuations to identify the glass transition temperature for a coarse-grained weakly semi-flexible polymer model. More precisely, we used principal component analysis (PCA) to quantify the conformational fluctuations and identify a sharp change in fluctuation around the glass transition temperature. The first eigen value of PCA shows a clear difference below and above glass transition temperatures. The new method of glass transition temperature predicted from PCA considers local structural fluctuations and does not depend on any fitting parameters like the existing methods.

CPP 9.4 Mon 15:45 H39

Systematic parametrization of non-Markovian dissipative thermostats for coarse-grained molecular simulations with accurate dynamics — •Viktor Klippenstein and Nico F. A. Van Der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The Mori-Zwanzig theory, in principle, allows to derive an exact equation of motion for coarse-grained degrees of freedom based on the dynamics of an underlying fine-grained reference system.[1] Still, in practice the simultaneous representation of structural and dynamic properties in particle-based models poses a complicated problem, e.g. due to the non-linearity of the exact coarse-grained equation of motion.

A viable approximate approach is to start from a conservative coarse-grained force-field and to extend the standard Newtonian equation of motion used in molecular simulation with a linear generalized Langevin thermostat. We demonstrate how such a thermostat can be parametrized to correctly represent dynamic properties, both in a purely bottom-up approach[2,3] or by applying iterative optimization.[3] We consider the Asakura-Oosawa model as a simple test case.[3]

[1] V. Klippenstein, M. Tripathy, G. Jung, F. Schmid, and N. F. A. van der Vegt, The Journal of Physical Chemistry B 125, 4931 (2021).

[2] V. Klippenstein and N. F. A. van der Vegt, The Journal of Chemical Physics 154, 191102 (2021).

[3] V. Klippenstein and N. F. A. Van Der Vegt, The Journal of Chemical Physics under review (2022).

CPP 9.5 Mon 16:00 H39

Stretching biopolymers with fluctuating bending stiffness — •Panayotis Benetatos — Kyungpook National University, Daegu, South Korea

In many biopolymers, the local bending stiffness fluctuates. For example, DNA-binding proteins attach to and detach from DNA to regulate cellular functions, thus causing a change in the local bending stiffness of the polymer backbone. This could also happen due to internal conformational transitions, such as the DNA denaturation or the helix-coil transition in polypeptides. What all these cases have in common is that the change in the local flexibility is transient and reversible. In order to analyse the conformational and elastic behaviour of such biopolymers, we propose a minimal but encompassing model of a freely jointed chain with reversible hinges (rFJC). We show that the tensile response of a rFJC is remarkably different from that of the usual freely jointed chain (uFJC). At small stretching forces, the rFJC is more compliant than the uFJC and the size (mean square end-to-end distance) of the former is greater than that of the latter. At strong stretching forces, in contrast, the rFJC is much stiffer than the uFJC. In this talk, we also discuss a strongly stretched wormlike chain with fluctuating local bending stiffness. We show that, under certain conditions, we get significant ensemble inequivalence (Gibbs vs Helmholtz).

CPP 9.6 Mon 16:15 H39

Modulating internal transition kinetics of responsive macromolecules by collective crowding — •Nils Göth, Upayan Baul, Michael Bley, and Joachim Dzubiella — Applied Theoretical Physics—Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

Packing and crowding are used in biology as mechanisms to (self-) regulate internal molecular or cellular processes based on collective signaling. Here, we study how the transition kinetics of an internal “switch” of responsive macromolecules is modified collectively by their spatial packing. We employ Brownian dynamics simulations of a model of Responsive Colloids, in which an explicit internal degree of freedom–here, the particle size–moving in a bimodal energy landscape self-consistently responds to the density fluctuations of the crowded environment. The bimodal energy landscape is motivated by existing two-state behavior like in protein folding or hydrogels with bimodal volume transitions. We demonstrate that populations and transition times for the two-state switching kinetics can be tuned over one order of magnitude by “self-crowding”. An exponential scaling law derived from a combination of Kramers' and liquid state perturbation theory is in very good agreement with the simulations.

[1] Upayan Baul, NG, MB, and JD, J. Chem. Phys. 155, 244902 (2021).

15 min. break

CPP 9.7 Mon 16:45 H39

Modelling process-structure-properties of polymer nanocomposites — •Janett Prehl, Constantin Huster, and Karl Heinz Hoffmann — TU Chemnitz, Chemnitz, Germany

Twin polymerization is a complex chemical reaction process leading to a broad range of organic-inorganic nano composite materials.

Within this presentation we will show our latest results [1] on the theoretical analysis of the structure formation process of twin polymerization via a previously introduced lattice-based Monte Carlo method, the reactive bond fluctuation model [2]. We analyze the effects of various model parameters, such as movability, attraction, or reaction probabilities on structural properties, like the specific surface area, the radial distribution function, the local porosity distribution, or the total fraction of percolating elements.

From these examinations, we may identify structural key factors and thus chemical properties of the underlying components that need to be adapted to fulfill desired requirements for possible applications.

[1] Prehl, J. and Huster, C., *polymers* **11** (2019) 878

[2] Hoffmann, K.H. and Prehl, J., *Reac. Kinet. Mech. Cat.* **123** (2018) 367-383; Huster, C., Nagel, K., Spange, S., and Prehl, J., *Chem. Phys. Lett.* **713** (2018) 145-148

CPP 9.8 Mon 17:00 H39

A cosolvent surfactant mechanism affects polymer collapse in miscible good solvents — •Swaminath Bharadwaj[1], Divya Nayar[1,2], Cahit Dalgicdir[1], and Nico van der Vegt[1] — [1]Technische Universität Darmstadt, Germany — [2]IIT Delhi, India

The coil-globule transitions of aqueous polymers are of profound significance in understanding the structure and function of responsive soft matter. In particular, the remarkable effect of amphiphilic cosolvents (which preferentially adsorb on the polymer surface) that leads to both swelling and collapse of stimuli responsive polymers is still hotly debated in the literature [1]. The predominant focus has been on the attractive polymer-(co)solvent interactions and the role of solvent-excluded volume interactions has been largely neglected. The solvent-excluded volume contribution to the solvation free energy corresponds to the formation of a repulsive polymer-solvent interface.

Using MD simulations, we herein demonstrate that alcohols reduce the free energy cost of creating a repulsive polymer-solvent interface via a surfactant-like mechanism which surprisingly drives polymer collapse at low alcohol concentrations. This hitherto neglected role of interfacial solvation thermodynamics is common to all coil-globule transitions [2], and rationalizes the experimentally observed effects of higher alcohols and polymer molecular weight on the coil-to-globule transition of thermoresponsive polymers [2]. This mechanism is generic and applicable to other solutions containing amphiphilic cosolvents or cosolutes.

References: [1] S. Bharadwaj et al., Soft Matter, 2022, 18, 2884. [2] S. Bharadwaj et al., Commun. Chem., 2020, 3, 165.

CPP 9.9 Mon 17:15 H39

Water transport in soft nanoporous materials: Impact of mechanical response on dynamics, slippage and permeance — •Alexander Schlaich[1,2], Matthieu Vandamme[3], Marie

Plazanet[2], and Benoit Coasne[2] — [1]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Germany — [2]Univ. Grenoble Alpes, CNRS, LIPhy, 38000 Grenoble, France — [3]Navier, Ecole des Ponts, Univ. Gustave Eiffel, CNRS, Marne-la-Vallee, France

Transport of water in soft porous materials is relevant to applications such as ultrafiltration and reverse osmosis processes, where polymeric membranes are employed in filtration/separation, or energy related processes. While water transport in hard porous materials such as porous silica glasses is well studied, the situation in soft matter is much more puzzling and remains unclear due to the combination of surface heterogeneity, the diffuse boundary location and pore deformations due to mechanical stresses.

In this work we study water in chemically realistic hydrophobic pores at different thermodynamic and mechanical conditions using atomistic molecular dynamics simulations. In detail, we analyze pore swelling, adsorption and confinement effects as well as microscopic diffusion mechanisms and transport effects due to pore size fluctuations. Strikingly, we find that hydrodynamic continuum models remain valid for planar flow of water even in monolayer confinement in soft pores.

CPP 9.10 Mon 17:30 H39

Solvation structure of polymer cathodes for Li/S batteries — •Diptesh Gayen[1], Yannik Schuetze[2], Sebastien Groh[1], and Joachim Dzubiella[1] — [1]Institute of Physik, University of Freiburg, Freiburg, Germany — [2]Helmholtz Zentrum Berlin, Berlin

Lithium-sulfur (Li/S) batteries are regarded as one of the most promising next-generation energy storage devices. Meanwhile, some challenges inherent to Li/S batteries remain to be solved, for instance, the polysulfide shuttle effect and the volume expansion of the cathode during discharge. To suppress the above-mentioned drawbacks, polymeric cathodes, e.g., based on poly(4-(thiophen-3-yl) benzenethiol) (PTBT) are considered sulfur host material (S/PTBT). Here, we use molecular dynamics (MD) computer simulations to study the structure and dynamics of a single PTBT chain at 300 K in different concentrations and compositions of dimethoxyethane (DME) and dioxolane (DOL) solvents. The force-field parameters for this polymer were constructed based on the OPLS database, with missing parameters newly developed by us by benchmarking to density-functional theory calculations. We report results on polymer conformational behavior, solvent-specific adsorption, and thermodynamic properties such as the partial molar volume. Our results show that DOL is more absorbed at the PTBT compare to DME. We find no significant effect of the solvent on the structure factor of the polymer. Our simulation model enables future systematic studies of PTBT in various solvent mixtures, in particular electrolytes, for the optimizations of modern Li/S batteries.

CPP 10: 2D Materials 2 (joint session HL/CPP/DS)

Time: Monday 15:00–18:30 Location: H36

CPP 10.1 Mon 15:00 H36

On-demand light emission from helium ion induced defects in atomically thin $\mathbf{WS_2}$ — •Nina Pettinger, Ana Micevic, Alexander Hötger, Christoph Kastl, and Alexander Holleitner — TU Munich, Germany

Optically active defects created with a helium ion microscope (HIM) propose the possibility for structuring and tailoring quantum emitters on an atomistic scale [1]. We introduce the generation of positioned defects in encapsulated monolayer WS_2 with a HIM. The HIM induced defects exhibit sharp photoluminescence emission in the energy range of 1.55 to 1.79 eV.

[1] J. Klein and L. Sigl et al., ACS Photonics 8, 669 (2021).

CPP 10.2 Mon 15:15 H36

Concept of an all-optical THz near-field microscope for flakes of 2D materials — •Ahmad-Reza Etemadi, Sebastian Matschy, Ahana Bhattacharya, and Martin Mittendorff — Department of physics, University of Duisburg-Essen, 47057 Duisburg, Germany

While THz spectroscopy is an excellent tool to investigate the free charge carriers in many semiconducting materials, the long-wavelength is an inherent feature linked to a large spot size in the millimeter range, and thus large samples are required. Small flakes of two-dimensional materials exfoliated from bulk crystals are usually much smaller than the spot size of a conventional THz spectrometer. The direct detection of the THz signal in the vicinity of the flake gains the phase and amplitude information with a higher spatial resolution. This is accessible by placing the sample directly on top of an electro-optic crystal. Sampling the THz field at the flake position gives access to the complex conductivity and thus the carrier density as well as the carrier mobility. A frequency-doubled fiber laser with a pulse duration of about 80 fs at 780 nm is exploited to generate and sample the THz field. GaSe, and ZnTe are employed as electro-optic crystals. Here we present the current state of the near-field microscope and the first measurements of the spatial resolution. The experimental results are accompanied by rigorous modeling of the THz propagation within the electro-optic crystal.

CPP 10.3 Mon 15:30 H36

Ab initio description of valley-selective circular dichroism — •Maximilian Schebek[1], Yiming Pan[2], Cecilia Vona[1], Claudia Draxl[1], and Fabio Caruso[2] — [1]Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

By enabling control of valley degrees of freedom, valley-selective circular dichroism (VSCD) has become a key concept in valleytronics. In this work, we present an *ab initio* many-body theory of VSCD based on the Bethe-Salpeter equation. Our approach provides a new route to accurately predict the degree of valley polarization upon absorption of circularly polarized light. With the example of monolayer transition-metal dichalcogenides, we further show that valley excitons - bound electron-hole pairs formed at either the K or $\overline{\mathrm{K}}$ valley upon absorption of circularly-polarized light - are chiral quasiparticles characterized by a finite orbital angular momentum (OAM). Beside governing the interaction with circularly polarized light, the OAM results in a finite magnetization of excitons, which in turn provides a route for the interaction of excitons with external magnetic fields and other spin-orbital degrees of freedom.

CPP 10.4 Mon 15:45 H36

Dark and bright exciton dynamics probed by time-resolved photoluminescence in hBN-encapsulated $\mathbf{MoWSe_2}$ monolayers — •Julian Schröer[1,3], Joanna Kutrowska-Girzycka[2], Leszek Bryja[2], Joanna Jadczak[2], and Jörg Debus[1] — [1]TU Dortmund, Experimentelle Physik 2, AG Debus — [2]Wroclaw University of Science and Technology, Department of Experimental Physics — [3]Universität Rostock, Institut für Physik, AG Korn: Zweidimensionale Kristalle und Heterostrukturen

Semiconducting monolayers of ternary $MoWSe_2$ alloys combine the unique properties of the binary transition metal dichalcogenide (TMDC) materials $MoSe_2$ and WSe_2. The alloying leads to, for example, brightening of the momentum- and spin-forbidden dark exciton states. Detailed studies on the dynamics of these brightened dark states are missing. We report on the exciton and trion formation lying in the 1-3 ps range, while the decay time approaches hundreds picoseconds. Additionally, strong dependences on the temperature and exciting laser light polarization are observed. In time-resolved and stationary photoluminescence measurements, we reveal the impact of the crystal disorder potential on the exciton properties. The polarization dynamics of the exciton and trion photoluminescence indicate possible contributions from chiral phonons as well as electrons and holes from different valleys of the Brillouin zone. Our work is a further step towards a deeper understanding of the dynamics of dark excitons in TMDC materials.

15 min. break

CPP 10.5 Mon 16:15 H36

Signatures of a degenerate many-body state of interlayer excitons in a van der Waals heterostack — •Johannes Figueiredo[1], Lukas Sigl[1], Florian Sigger[1], Jonas Kiemle[1], Mirco Troue[1], Ursula Wurstbauer[2], and Alexander Holleitner[1] — [1]Walter-

Schottky-Institut, Technical University of Munich — [2]Institute of Physics, Westfälische Wilhelms-Universität Münster

In atomistic van der Waals heterostacks of transition metal dichalcogenides, the reduced dimensionality and changing dielectric environement leads to the formation of stronlgy bound excitons. Optically generated interlayer excitons exhibit an additional spatial separation of the electron-hole pair with a reduced overlap of the electrons' and holes' wave-functions, evidenced through their long lifetimes. These long-lived, photogenerated composite bosons yield several signatures of a quantum degenerate many-body system at cryogenic temperatures. The emergence of this state is in accordance with theoretical predictions of a critical condensation temperature above 10K. We present new insights into the phase-diagram of such interlayer exciton ensembles. [1]
[1] L. Sigl *et al.*, Phys. Rev. Research 2, 042044(R) (2020)

CPP 10.6 Mon 16:30 H36

exciton species in highly doped WS_2 monolayers — david tiede, •hossein ostovar, hendrik lambers, nihit saigal, and ursula wurstbauer — Institute of Physics, University of Münster, Münster, Germany

Semiconducting two-dimensional transition metal dichalcogenides such as WS_2 excel due to their exciton dominated light-matter interaction even at room temperature (RT) that is highly tunable by external stimuli such as doping, light excitation, dielectric environment, or strain [1]. In this work, an optimized field effect structure utilizing a polymer electrolyte top gate electrode is employed to study the evolution of the optical response in monolayer WS_2 at RT in dependence of doping by means of photoluminescence and spectroscopic imaging ellipsometry measurements. The huge geometrical gate capacitance enables capacitance spectroscopy of the conduction band as well as valence band edge yielding a gap energy of 2.6eV in agreement with the determination from the exciton Rydberg series. The gate allows the injection of large electron and hole densities exceeding $10^{14}cm^{-2}$, sufficient to enable the exciton Mott transition. The obtained doping dependent emission and absorption spectra also facilitate the identification of phonon activated, neutral and charged exciton species as well as dressed excitons in a fermi sea. We acknowledge financial support via DFG WU 637/7-1 and SPP2244. [1] U. Wurstbauer et al. J. Phys. D: Appl. Phys. 50, 173001 (2017).

CPP 10.7 Mon 16:45 H36

Pump probe signatures of interlayer excitons in TMDC heterostructures — •Henry Mittenzwey, Manuel Katzer, Andreas Knorr, and Malte Selig — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

TMDC heterobilayers are promising candidates for novel optoelectronic applications, since they exhibit long-lived excitonic states with spatially separated electrons and holes located in different layers. The relaxation dynamics of these interlayer excitons and their interplay with intralayer excitons are still under investigation.

Here, we present a microscopic description for the phonon and tunneling induced formation and relaxation of intra- and interlayer excitons in a MoSe$_2$/WSe$_2$ stack. Based on the microscopic dynamics we calculate the pump probe signal for intra- and interlayer transition and their population dynamics including hot exciton bottleneck effects.

CPP 10.8 Mon 17:00 H36

Angle- and polarization-resolved luminescence from suspended and hBN encapsulated MoSe$_2$ monolayers — •Bo Han[1], Sven Stephan[1], Joshua J.P. Thompson[2], Martin Esmann[1], Carlos Antón-Solanas[1], Hangyong Shan[1], Samuel Brem[3], Christoph lienau[1], Kenji Watanabe[4], Takashi Taniguchi[4], Martin Silies[1], Ermin Malic[2,3], and Christian Schneider[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Philipps Universität, Marburg, Germany. — [3]Chalmers University of Technology, Gothenburg, Sweden. — [4]National Institute for Materials Science, Tsukuba, Japan.

We apply combined angle- and polarization-resolved spectroscopy to explore the interplay of excitonic physics and phenomena arising from the commonly utilized encapsulation on the optical properties of atomically thin transition metal dichalcogenides. In our study, we probe MoSe$_2$ monolayers which are prepared in both a suspended and an encapsulated manner. We show that the hBN encapsulation significantly enhances the linear polarization of exciton PL at large emission angles. This degree of linear polarization of excitons can increase up to 17 % in the hBN encapsulated samples. As confirmed by finite-difference time-domain simulations, it can be directly connected to the optical anisotropy of the hBN layers. In comparison, the linear polarization at finite exciton momenta is significantly reduced in suspended MoSe$_2$ monolayer, and only becomes notable at cryogenic conditions. This phenomenon strongly suggest that the effect is rooted in the k-dependent anisotropic exchange coupling inherent in 2D excitons.

15 min. break

CPP 10.9 Mon 17:30 H36

Photonic and Phononic Couplings in Hybrid High-Q Nanocavities with Encapsulated MoS2 Monolayer — •Chenjiang Qian[1], Viviana Villafañe[1], Pedro Soubelet[1], Alexander Hötger[1], Takashi Taniguchi[2], Kenji Watanabe[2], Nathan Wilson[1], Andreas Stier[1], Alexander Holleitner[1], and Jonathan Finley[1] — [1]Walter Schottky Institut and Physik Department, Am Coulombwall 4, 85748 Garching, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

Monolayer TMDs are ideal active materials for solid-state cQED. However, the direct cou-pling of TMDs to 0D nanocavities whilst preserving pristine excitonic properties and large cavi-ty-TMD overlap remains a challenge. Most commonly, non-encapsulated TMDs are stacked on top of prefabricated photonic structures using pick-and-place assembly. In this case, environ-mental disorders strongly perturb the excitonic properties. Whilst disorder can be mitigated by full hBN encapsulation, this approach moves the TMD away from the cavity field, thereby, trad-ing spatial coupling for homogeneous linewidth. Here, we integrate hBN/MoS2/hBN heterostruc-tures to Si3N4 nanobeams as hybrid nanocavities. Our approach solves the trade-off problem by making the unpatterned heterostructure a functional part of the cavity field. Therefore, the pris-tine excitonic quality, high cavity mode Q-factor $>$ 10000, and the strong cavity-MoS2 overlap are achieved simultaneously. We study the coupling of MoS2 excitons to the cavity optical and vibrational modes using PL and Raman spectroscopy, and novel coupling phenomena are ob-served based.

CPP 10.10 Mon 17:45 H36

Terahertz free carrier absorption to modulate the optical properties of nanometer-thick van der Waals semiconductors — •Tommaso Venanzi[1,2], Malte Selig[3], Alexej Pashkin[2], Stephan Winnerl[2], Manuel Katzer[3], Himani Arora[2], Artur Erbe[2], Amalia Patane[4], Zakhar R. Kudrynskyi[4], Zakhar D. Kovalyuk[5], Leonetta Baldassarre[1], Andreas Knorr[3], Manfred Helm[2], and Harald Schneider[2] — [1]Sapienza University of Rome, 00185 Rome, Italy — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Technical University Berlin, 10623 Berlin, Germany — [4]University of Nottingham, Nottingham NG7 2RD, UK — [5]The National Academy of Sciences of Ukraine, 58001 Chernivtsi, Ukraine

Free carriers in doped semiconductors absorb terahertz radiation when the frequency of the electromagnetic field is lower or comparable to the plasma frequency of the system. This phenomenon can be used to manipulate the optical response of the material. We present here the results of two different experiments performed at the infrared free-electron laser FELBE on atomically-thin van der Waals semiconductors. In MoSe2 monolayers, we observe a terahertz-induced redshift of the trion resonance. Terahertz absorption induces an average high momentum to the carriers and this momentum gets transferred during the trion formation, resulting in a net redshift in the absorption. In few-layer InSe, the terahertz pulses induce a transient quenching of the photoluminescence emission. In both cases, a microscopic study of the hot carrier distribution cooling is also presented.

CPP 10.11 Mon 18:00 H36

Theory of Exciton-Phonon Interaction for Stationary State Experiments in Atomically Thin Semiconductors — •Manuel Katzer, Andreas Knorr, and Malte Selig — Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Atomically thin semiconductors exhibit tightly bound electron hole pairs which stimulated exciton research in recent years [1]. While typical experimental techniques include the cw excitation of the material, only few is known theoretically about the related exciton dynamics and the formation of non-equilibrium steady states. Based on excitonic

Boltzmann scattering equations, we demonstrate that the formation of such stationary states is also accompanied with the formation of phonon replica in the photoluminescence excitation spectrum [2], in agreement with available experiments [3]. So far, many studies focused on the understanding of exciton dynamics in the limit of weak excitation. Above this limit, we find both bosonic but also fermionic contributions to the thermalization, due to the co-bosonic nature of excitons. Based on a Heisenberg equation of motion ansatz [4], we discuss the first order of non-linear exciton-phonon interaction exceeding the classical Boltzmann scattering limit, in order to analyze the exciton thermalization at elevated excitation densities.
[1] Wang et al. RMP, 90, 021001 (2018). [2] Selig et al. arXiv:2201.03362 (2022). [3] Chow et al., Nano lett. 17, 1194 (2017); Shree et al. PRB 98, 035302 (2018). [4] Selig et al. PRR, 1, 022007 (2019); Katsch et al., PRL 124 25 257402 (2020).

CPP 10.12 Mon 18:15 H36

Ultrafast control of spins in transition metal dichalcogenides — •Abhijeet Kumar[1], Denis Yagodkin[1], Douglas J. Bock[1], Nele Stetzuhn[1,2], Sviatoslav Kovalchuk[1], Alexey Melnikov[3], Peter Elliott[2], Sangeeta Sharma[2], Cornelius Gahl[1], and Kirill I. Bolotin[1] — [1]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany — [2]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born Straße 2a, 12489 Berlin, Germany — [3]Institute for Physics, Martin Luther University Halle, 06120 Halle, Germany

Control and manipulation of the coupled spin/valley degrees of freedom in transition metal dichalcogenides (TMDs) are essential for their applications in spin/valleytronics. Here, we achieve ultrafast control of spins in TMDs via two distinct approaches, namely, proximity-coupling to another TMD and strain. First, we use a type-II heterostructure MoS_2-MoSe_2 to enable directional optical pumping of spin-polarized carriers. We find that the photoexcited carriers conserve their spin for both tunneling directions across the interface. We observe dramatic differences in the spin/valley depolarization rates for electrons and holes, 30 and <1 ns^{-1}, respectively, which relates to the disparity in the spin-orbit splitting in conduction and valence bands of TMDs. Second, by applying biaxial strain (exceeding 2%) in monolayer WSe_2, we evidence the hybridization of the conduction bands with the in-gap localized defects that brightens the lowest-lying dark excitons. This novel hybrid state exhibits unique spin/valley signatures which are strongly manipulated on picosecond-timescale by strain and doping.

CPP 11: 2D Materials 3 (joint session CPP/DS)

Time: Monday 17:15–17:45 Location: H38

CPP 11.1 Mon 17:15 H38

On the electronic pi-system of 2D covalent organic frameworks — •Konrad Merkel, Johannes Greiner, and Frank Ortmann — TU München

We investigate a family of 2D hexagonal covalent organic frameworks (COFs) with different linker monomers regarding their electronic structure and pi-conjugation. Molecular orbitals can be obtained from maximally localized Wannier functions and turn out to be sigma- and pi-like orbitals forming distinct sigma- and pi-bands, respectively. The Wannier description enables a detailed analysis of the topology, effective coupling and delocalization of the entire pi-system. We identify conjugated states that are delocalized across multiple building blocks of the COF and show their robustness against perturbations like out-of-plane rotations of molecular fragments and different strength of Anderson disorder. Furthermore, we apply the nucleus-independent chemical shift (NICS), which is an established measure of aromaticity. All results are compared for different types of linker units with different degrees of pi-conjugation.

CPP 11.2 Mon 17:30 H38

Permeation of gases through molecularly thin carbon nanomembranes — •Vladislav Stroganov[1], Daniel Hüger[1], Tabata Nöthel[1], Christof Neumann[1], Uwe Hübner[2], Michael Steinert[1], Monika Kruk[3], Piotr Cyganik[3], and Andrey Turchanin[1] — [1]Friedrich-Schiller University Jena, Jena, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany — [3]Jagiellonian University, Kraków, Poland

Atomically thin carbon nanomembranes (CNMs) are promising candidates for next generation filtration and gas separation technologies. However, the gas permeation mechanism through CNMs is not fully understood yet. To improve this knowledge, we investigated permeation of helium, deuterium, water vapor and other gases through a series of CNMs under different conditions. The CNMs were synthesized from biphenyl substituted carboxylic acids on silver substrate $C_6H_5-C_6H_4-(CH_2)_n-COO|Ag$, with different lengths of aliphatic linker n = 2 - 6. A CNM based on terphenyl thiol (TPT) was used as a well-known reference system. We demonstrated that even the smallest variation in the structure of the molecular precursor lead to significant change of the permeation properties.

CPP 12: Poster 1

Active Matter (12.1-12.2), Biopolymers, Biomaterials and Bioinspired Functional Materials (12.3-12.9), Charged Soft Matter, Polyelectrolytes and Ionic Liquids (12.10-12.15), Complex Fluids and Colloids, Micelles and Vesicles (12.16-12.19), Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods (12.20-12.22), Modeling and Simulation of Soft Matter (12.23-12.28), Responsive and Adaptive Systems (12.29-12.35), Wetting, Fluidics and Liquids at Interfaces and Surfaces (12.36-12.39), Electrical, Dielectrical and Optical Properties of Thin Films (12.40-12.41), Hybrid and Perovskite Photovoltaics (12.42-12.54), Molecular Electronics and Excited State Properties (12.55-12.58), Organic Electronics and Photovoltaics (12.59-12.80)

Time: Monday 18:00–20:00 Location: P1

CPP 12.1 Mon 18:00 P1

Janus particles: Challenges in the preparation process and analysis of their thermophoretic self-propulsion — •Franziska Jakob and Regine von Klitzing — Institute for Condensed Matter Physics, Technische Universität Darmstadt, D-64289 Darmstadt

Active colloidal particles with different functionalities at their opposite sides are named Janus particles - motivated by the Roman mythological god. One possible propulsion mechanism is thermophoretic self-propulsion. When laser light ($\lambda = 532$ nm) illuminates a gold-capped particle, a local temperature gradient is generated along the particle surface due to surface plasmon excitation of the gold cap. This gradient perturbs the equilibrium conditions of the surrounding medium and finally leads to particle self-propulsion.

This contribution focuses on various preparation processes of self-thermophoretic gold-polystyrene (Au-PS) microswimmers. The influence of the preparation technique on the gold cap size and the resulting self-thermophoretic behavior of the Janus particle will be presented. For this purpose, Janus particles are prepared either by metal sputtering, thermal evaporation, or by a combination of gel trapping technique and metal sputtering. With scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX), the dimension of the gold cap was investigated. Dark-field microscopy (DFM) combined with a LabView program enables real-time tracking of the Janus particles. The study shows that the preparation method strongly affects the gold cap size of the Janus particles and thus influences their self-thermophoretic velocity.

CPP 12.2 Mon 18:00 P1

Modeling Chemotaxis and Cross-Diffusion using MD and cDFT — •Philipp Stärk — SC Simtech, Uni Stuttgart, Germany

Multiple experimental studies have observed diffusion of certain particle types—such as catalysts—along concentration gradients of other species. Using stochastic, coarse grained reaction dynamics in MD simulations, we present simplified models for this behavior. Furthermore, we present a classical Density Functional Theory which provides a simple model for cross-diffusion on a broader class of particle types.

CPP 12.3 Mon 18:00 P1

Cellulose-based programmable, robust, and healable actuators for smart packaging devices — •Qing Chen[1], Benedikt Sochor[1], Andrei Chumokov[1], Marie Betker[1,2], Nils Ulrich[3,4], Maria E. Toimil-Molares[4], Korneliya Gordeyeva[2], Daniel Söderberg[2], Volker Körstgens[5], Matthias Schwartzkopf[1], Peter Müller-Buschbaum[5], and Stephan Roth[1,2] — [1]DESY, 22607 Hamburg, Germany — [2]KTH, 10044 Stockholm, Sweden — [3]GSI Helmholtz Center, 64291, Darmstadt, Germany — [4]TU Darmstadt, 64287 Darmstadt, Germany — [5]TU Munich, 85748 Garching, Germany

Programmable actuators are promising candidates for smart devices. Herein, we fabricated a cellulose-based actuator with polyvinyl alcohol (PVA) and polystyrene sulfonate (PSS) as reinforcement. Driven by moisture, the actuators bend in programmable directions when we cut the films at different oblique angle with respect to its radial axis. Furthermore, the actuator shows an exceptional elongation-at-break of 77%. Ultra-Small-Angle X-ray Scattering and scanning electron microscopy examination at the necking region of the film yields the formation of cavities with an average width of 75 nm. They decrease to 16.5 nm with an elevating relative humidity (RH) from 0 to 100% and remains constant when the RH decreases from 100% to 0%. The programmable, robust, and healing ability of the actuator suggests its potential as smart packaging devices.

CPP 12.4 Mon 18:00 P1

A Raman spectroscopic study of the pyrolysis of lactose and tannins — •Simon Brehm, Cameliu Himcinschi, Jakob Kraus, and Jens Kortus — TU Bergakademie Freiberg, Germany

Lactose and tannin are naturally occurring and eco-friendly alternatives to commonly used binders for carbon-bonded alumina filters that are applied in steel melt filtration. A contribution to understand the production process of these filters is the investigation of the pyrolysis process of the binders. In this work, lactose and different tannins were investigated by *in situ* and *ex situ* Raman spectroscopy. The transformation of the tannin and lactose molecules to a system of amorphous carbon and at even higher temperatures to nanocrystalline graphite could be observed in the Raman spectra. In addition, intermediate pyrolysis products of the investigated tannins as well as their pyrolysis temperatures could be determined.

CPP 12.5 Mon 18:00 P1

F-Actin photocleavage as an artificial secondary nucleation model — •Stephan Sydow, Tobias Thalheim, Jörg Schnauss, and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Leipzig, Germany.

The aggregation of soluble proteins into highly ordered, insoluble amyloid fibrils is characteristic for a range of neurodegenerative disorders, like Alzheimer's or Parkinson's disease. The kinetics in the formation of amyloid fibrils are governed by multiple aggregation mechanisms, which are present simultaneously. One of these being the unspecific spontaneous breaking of Amyloid fibrils, whose cause, rate and break size distribution are still unknown, due to them being hidden in ensemble measurements.

We employ an artificial model system with a controllable fragmentation rate to compare it with current amyloid kinetic models, all assuming a homogeneous break size distribution. Fluorescence labelled Actin filaments exhibit photocleavage. By laser illumination of single, homogeneously labelled filaments in solution, we are able to control the breakage rate. The length and position of filaments and fragments are imaged over time by fluorescence microscopy.

We show, that Actin filaments exhibit a homogeneous break size distribution, verifying our artificial model system. Additionally, the fragment size distribution is independent of the intensity dependent, induced cleavage rate, thus it enables the direct comparison to current amyloid models.

CPP 12.6 Mon 18:00 P1

Mapping nanomechanics and energy dissipation of collagen fibrils in tendon — •Martin Dehnert, Paul Zech, Mario Zerson, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

We study the nanomechanical properties of hydrated collagen fibrils with AFM-based nanoindentation measurements. Force–distance (FD) data measured with tip velocities $< 1\,\mu$m/s display a rate-independent hysteresis with return point memory depending on only one return point. With different indentation protocols, we show that stress relaxation and creep do not influence the time evolution of the FD data. The main cause of hysteresis is the elastoplastic deformation of collagen fibrils above the glass transition. We explore the variations of these nanomechanical properties in sets of unfixed hydrated collagen fibrils isolated from native chicken Achilles tendon and compare them with collagen fibrils embedded in the natural tendon. AFM imaging in the air with controlled humidity preserves the tissue's native water content and allows for high-resolution imaging and nanoindentation measurements. This sheds new light on the role of interfibrillar bonds, the mechanical properties of the interfibrillar matrix, and the biomechanics of native tendon.

CPP 12.7 Mon 18:00 P1

Hydrogel-based electrodes for brain wave detection — •Gökay Erbil[1], Hsin-Yin Chiang[2], Volker Körstgens[1], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Cephalgo, 75014 Strasbourg, France

Electroencephalography (EEG) as method for detecting brain waves is gaining importance for medical applications, since it can non-invasively provide information. Currently, both wet electrodes and dry electrodes are in use for clinical and commercial applications. With both concepts, one has to deal with certain challenges. Dry electrodes often show motion artifacts due to changes in contact and pressure applied between skin and electrode altering the signal quality. For wet electrodes on the other hand, a decrease in signal quality is usually observed with long term signal acquisitions. In this work, mussel inspired hydrogels are presented to address these challenges. The hydrogel electrodes containing tannic acid and silver nanoparticles are optimized in terms of high conductivity and adhesive properties. The elevation of brain waves collected with a headset comprised of hydrogel electrodes is demonstrated in an EEG setup for long term analysis.

CPP 12.8 Mon 18:00 P1

Spin-Based Quantum Sensing with Endohedral Fullerenes — •Marco Sommer[1], Don-Sheng Guo[1], Andreas Hennig[1], Johann P. Klare[1], and Wolfgang Harneit[2] — [1]Universität Osnabrück, Osnabrück, Deutschland — [2]Nankai University, Tianjin, China

The endohedral fullerene N@C_{60} in an inhomogeneous environment is investigated with the goal to establish the N@C_{60} with its outstanding spin properties as a spin label for coupling experiments in biological systems at room temperature. To reveal the preservation of these spin features, the N@C_{60} is transferred into Triton X-100 micelles, a deep cavitand calixarene (SAC4A) as well as the cavity formed by two γ-cyclodextrins building a non-covalently bonded guest-host complex. The spectroscopic tools are based primarily on continuous wave (cw) and pulsed electron paramagnetic resonance (EPR) techniques, in addition to absorption measurements in the ultraviolet-visible light (UV/vis) range and molecular modelling with molecular dynamic (MD) simulation of the complexes. The resulting spin properties are examined with cw and pulsed EPR spectroscopy. The computational modelling and MD simulations of the complexes in combination with UV/vis spectroscopy serves for the unravelling of the arrangement. Initial experiments show a successful transfer of the highly hydrophobic N@C_{60} into the aqueous phase. The resulting spin-spin relaxation time T_2 strongly depends on the the N@C_{60}'s encapsulation system. Inhomogeneous environments (Triton X-100) decrease the transverse relaxation time whereas a symmetric system (γ-cyclodextrin) provides an increase in T_2.

CPP 12.9 Mon 18:00 P1

Studying the nanomechanical properties of functional organic and biologic macromolecules — Ilka M. Hermes[1], Andrea Cerrata[2], Vladimir Korolkov[2], and •Alexander Klasen[2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Park Systems Europe GmbH, Mannheim, Germany

As the functionality of organic and biologic macromolecules is often determined by their nanomechanical properties, visualizing the distribution of mechanical properties on the nanoscale provides crucial insights for soft matter research. [1,2] Here, we present a study on structural and nanomechanical properties of functional organic and biologic macromolecules in different environments as well as under external stimuli, such as temperature, ion concentration and pH. Force-distance measurements with atomic force microscopy (AFM) resolve adhesion and elasticity by pressing a nanometer-sized tip on the end of a cantilever onto the surface. However, the correlation of mechanical data from force-distance measurements to the local sample morphology additionally requires topographic sample information. PinPointTM nanomechanical imaging simultaneously acquires topographic and force-distance data within short amounts of time and is therefore ideally suited to investigate organic and biologic macromolecules.

1. S. Perni et al., Langmuir 32, 7965-7974 (2016).
2. E. E. Bastounis et al., Mol. Biol. Cell 29, 1571-1589 (2018).

CPP 12.10 Mon 18:00 P1

Huge pKa-Shifts in Weak Polyelectrolyte Brushes Explained by Coarse-Grained Simulations — •David Beyer[1], Christian Holm[1], and Peter Košovan[2] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czechia

Following recent experiments, we study the titration behaviour of weak (pH-responsive) polyelectrolyte brushes at different salt concentrations using coarse-grained computer simulations. To account for charge regulation and the exchange of small ions with the bulk solution, we make use of the Grand-Reaction Monte-Carlo method (G-RxMC). Our simulations yield ionization curves which strongly deviate from the ideal result. Furthermore, we observe a strong dependence of the deviation on the bulk salt concentration, amounting to a shift of approximately one unit of pH as the salt concentration decreases by one order of magnitude. We theoretically explain the observed titration behaviour as a consequence of the Donnan partitioning between the brush and the bulk solution. To confirm our theoretical explanation we measure the pH inside the brush, which eliminates the Donnan contribution. Our results show that the Donnan effect can account for a shift in pH between the bulk and the brush of more than 4 units in extreme cases. We finally plot the degree of ionization as a function of the pH inside the brush, thus eliminating the Donnan contribution. Up to a small shift due to the electrostatic interactions, the resulting curves almost coincide with the ideal result, thus confirming our hypothesis.

CPP 12.11 Mon 18:00 P1

Narrow Gap Flow Electrolysis Cells: Atomistic Computer Simulation of Electric Field Effects on Water/Organic Mixtures — •Anastasios Sourpis and Friederike Schmid — Johannes Gutenberg University, Mainz, Germany

Electrolyte-free electrolysis fuel cells are central to a sustainable future with clean water. With growing industrial development, for example, toxic heavy metals, radioactive ions, and inorganic compounds are increasingly discharged into the environment and our sources of drinking water. In novel cutting-edge developed electrolysis fuel cells [1] the case of electrolyte-free electrolysis has been observed for mixtures of water and acetonitrile. These high modular flow cells of electro organic synthesis are very promising for the production of fine chemicals and pharmaceutically active agents. The purpose of this study is to qualitatively and quantitatively evaluate the effect of electric fields on electrolysis cells. Especially in the case of acetonitrile and water mixtures, we have focused on understanding by atomistic simulations the existence of the electrical conductance and how this can be described on larger scales.

CPP 12.12 Mon 18:00 P1

Controlling the phase transitions in surfactant-dna complexes — A.V. Radhakrishnan[1,2], S. Madhukar[1], A. Choudhari[1], and •V.A. Raghunathan[1] — [1]Raman Research Institute Bangalore 560080 India — [2]Experimental Physics I, University of Bayreuth, Bayreuth 95447 Germany

Surfactant-DNA complexes are a special class of polyelectrolyte complexes where one of the macroions is formed by self assembly. They have been studied for their interesting electrostatics and potential applications for gene delivery and photonic applications. The gain in counter ion entropy is driving the complex formation and there is an interesting interplay of electrostatics and entropy leading to a rich phase behavior. The self assembled macroion can be formed either by a bilayer forming lipid or a micelle forming surfactant. We have studied the structural transitions in complexes formed by cationic surfactants such as CTAB, CTAT, DTAB with ds-DNA and constructed phase diagrams. Using small angle xray scattering and polarizing optical microscopy and elemental analysis the presence of a various phases, including a square phase(S), hexagonal phase (H) and a hexagonal super lattice phase (Hs) are identified. Detailed modeling of these structures have been carried out based on the electron density maps to propose the packaging of the macroions in the lattices. Striking differences in the phase diagrams and various ways of controlling the structural transitions will be discussed.

CPP 12.13 Mon 18:00 P1

Poly((trifluoromethane)sulfonimide lithium styrene) as single-ion conducting binder for lithium iron phosphate electrodes in lithium-ion batteries — •Fabian A.C. Apfelbeck[1], Julian E. Heger[1], Tianfu Guan[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik- Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]Royal Institute of Technology KTH, 100 44 Stockholm — [4]MLZ, TU München, 85748 Garching

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) represent a safe alternative to conventional electrolytes. Especially single-ion conducting polymers (SICPs), which have the anion covalently bonded to the backbone of the polymer and thus a theoretical transference number of unity, attracted strong interest in battery research. For full-cell performance investigation of these battery cells, the ion-conducting polymer electrolyte is often used as binder instead of the neutral polyvinylidenfluorid (PVDF) in order to enhance ion conduction in the electrode and decrease the interfacial contact. Here, lithium iron phosphate (LFP) cathodes with different weight ratios of PVDF and the SICP poly((trifluoromethane)sulfonimide lithium styrene) (PSTFSILi) as binders are prepared and analysed with real (scanning electron microscopy) and reciprocal (grazing-incidence small/wide angle x-ray scattering) space techniques.

CPP 12.14 Mon 18:00 P1

Influence of Li Salt concentration in poly(propylene carbonate) based solid polymer electrolytes — •Thien An Pham[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]MLZ, TU München, 85748 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Li metal exhibits a high specific capacity as well as a low discharge potential that makes it interesting as an anode material for Li ion batteries. But Li dendrite growth remains a major safety in cells with liquid electrolyte. Solid polymer electrolytes (SPE) show a higher mechanical stability in comparison to their liquid counterparts and thus, can inhibit dendrite growth. In order to achieve even higher energy densities, high-energy cathode materials such as Ni rich layered transition metal oxides should be combined with Li metal anodes. However, the high operation potentials of those cathodes are a challenge for SPE. Poly(propylene carbonate) (PPC) has an intrinsically high oxidation voltage exceeding 4.5 V making it suitable for high voltage operation. Here, SPE with PPC as polymer host and Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt are prepared and the influence of the salt concentration on the SPE properties are studied with electrochemical impedance spectroscopy and differential scanning calorimetry. Results have shown that the ionic conductivity increasing and the glass transition temperature is decreasing with higher amount of LiTFSI.

CPP 12.15 Mon 18:00 P1

Influence of Solvent and Lithium Salt on the Structure and Performance of NCM111 Cathode for Lithium Ion Batteries — •Yuxin Liang[1], Zhuijun Xu[1], Kun Sun[1], Tianfu Guan[1], Fabian Apfelbeck[1], Pan Ding[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Walter Schottky Institute, Experimental Semiconductor Physics, 85748 Garching — [3]MLZ, TU München, 85748 Garching

Lithium ion batteries (LIBs) with a wide range of applications have emerged as the most promising candidate for electrochemical energy storage due to its higher specific energies, volumetricenergy densities and power densities. However, lithium dendrite will growth and the Coulombic efficiency (CE) will decrease with Li plating and stripping. During past decades, more and more state-of-art materials has been developed to alleviate the abovementioned problems. Nevertheless, fundamental research on the component composition and the effect of additive and solvent on LIBs is still lacking. It is of great value to get a deep understanding and therefore optimize the fabrication process for future studies on the electrode/electrolyte interface of LIBs. In this project, we select the LiNi0.33Mn 0.33Co0.33O2 as cathode material to find out the effect of different solvents and extra lithium salt (LiTFSI) on the performance of LIBs. The Li/cathode cells were assembled to observe the battery performance and grazing incidence wide-angle X- ray scattering (GIWAXS) technique is used to detect structure change within the cathode before and after cycling.

CPP 12.16 Mon 18:00 P1

Scaling mechanical instabilities in drying micellar droplets — •Jayant Kumar Dewangan[1], Nandita Basu[2], and Mithun Chowdhury[1] — [1]Lab of Soft Interfaces, Metallurgical Engineering and Materials science, IIT Bombay, Mumbai 400076, India — [2]Department of Chemistry, IIT Bombay, Mumbai 400076, India

We present unique wrinkling patterns produced by evaporating sessile micellar aqueous droplets on rigid and soft substrates kept at temperatures far above ambient. The wrinkling patterns vary dramatically depending on the material's elastic modulus and substrate, the concentration of the micellar solution, and the temperature of the substrate. Coffee-ring-like morphologies are observed at very low concentration regimes (CTAB concentration < 0.0364 wt%), devoid of any wrinkling morphology, regardless of substrate temperature. Droplets deposited at a temperature above 85°C wrinkle formation begins at the droplet peripheral zone, radial on the stiff glass annular on soft cross-linked PDMS substrate, at the high initial concentration regime (CTAB concentration > 0.0364 wt%). Radial wrinkles on the glass substrate and annular wrinkles on the cross-linked PDMS substrate nucleate from the edges connecting to the deposit's central region at CTAB concentration > 2.73 wt%. The ratio of the width of the gel-like deposit to the radius of the droplet scales with surfactant concentration is dependent on the initial equilibrium contact angle of micellar droplets. Our findings support previous literature on mechanical instabilities of dried deposits by interdependent scaling relationships between deposit radius, wavelength of wrinkle, thickness, and elastic modulus.

CPP 12.17 Mon 18:00 P1

A scaled-down double-pass optical beam deflection setup for the measurement of diffusion and thermodiffusion in liquid mixtures — Mareike Hager, •Roman Reh, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

We report about a compact double-pass optical beam deflection (OBD) setup for measurments on diffusion and thermodiffusion in liquid mixtures. A laserbeam transmitted through the sample gets back-reflected behind the OBD-cell and, thus, traverses the sample volume a second time. Applying a vertical temperature gradient to the sample leads to thermodiffusion and the beam gets deflected by the resulting gradient in refractive index due to the gradients in temperature and concentration. A beamsplitter guides the beam towards a camera, where the time dependent laserposition is recorded. The signal then gives information about the diffusion processes. Since the laserbeam propagates on the same path between the beamsplitter and the cell before and after getting deflected in the sample and since the double-transmission geometry allows little distance between cell and camera, the whole setup could be built very compact. Measurements with different binary mixtures are in good agreement with measurements with a single-transmission-OBD. We present a matrix formalism to describe the optical transfer function of the instrument.

CPP 12.18 Mon 18:00 P1

Particle sorting by Marangoni convection in microfluidic channels — •Roman Reh, Lorenz Kiel, Daniel Zapf, and Werner Köhler — Physikalisches Institut, Universität Bayreuth, Germany

Thermosolutal and thermocapillary Marangoni convection at a liquid-gas interface in a T-shaped microchannel structure of approximately $100 \times 20\ \mu m^2$ cross section creates localized vortices that can be used for particle trapping, steering, and sorting. Experiments have been performed with water-ethanol mixtures as carrier liquid and dispersed micrometer-sized polystyrene beads. Due to collisions with the meniscus, particles are displaced from streamlines that approach the interface closer than one particle radius. These streamlines feed liquid volumes that are entirely cleared of particles. Particle accumulations structures form inside the vortex, from where only small particles can escape by diffusion. Since the critical streamline, which separates the depletion from the accumulation region, depends on the particle radius, the mechanism can be used for particle sorting by superposition of a Poiseuille flow and splitting of the flow downstream from the meniscus. In the simplest case, the initially homogeneous flow is split into two arms, one where the particles are enriched and one where all particles are removed from the liquid. The microchannel structures consist of crosslinked PDMS and the dispersed particles are observed by video microscopy. Numerical simulations are performed that almost perfectly match the experimental observations.

CPP 12.19 Mon 18:00 P1

Dynamic Ellipsometric Light Scattering: A Feasibility Study — •Reinhard Sigel — Markdorf, Germany

For colloidal particles dispersed in water, ellipsometric light scattering (ELS) has been established as a means for the characterization of the particles' interface layers [1,2]. These layers are important for the colloidal stabilization. We explore theoretically a combination of ELS with photon correlation measurements to access the fluctuation amplitude and dynamics of soft colloidal layers (e.g. in steric stabilization). They are connected to mechanical properties of the layers and are complementary to the structure information of conventional ELS. The investigation builds on preceding work on Mie scattering by soft core-shell particles [3], correlation ellipsometry [4], extraction of the coherent scattering properties in ELS for polydisperse samples [5,6], and the detection of incoherent dynamics in the ellipsometry minimum [7].

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[3] D. J. Ross, R. Sigel, Phys. Rev. E 85, 056710 (2012)

[4] R. Sigel, Soft Matter 13, 1132-1141 (2017)

[5] R. Sigel, A. Erbe, Appl. Opt. 47, 2161-2170 (2008)

[6] A. Erbe, K. Tauer, R. Sigel, Langmuir 25, 2703-2710 (2009).

[7] A. Erbe, R. Sigel, Phys. Chem. Chem. Phys. 15, 19143-19146 (2013)

CPP 12.20 Mon 18:00 P1

Improved virtual orbitals for charge transfer excitations in time dependent DFT — •Rolf Würdemann[1] and Michael Walter[2,3] — [1]Freiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — [3]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

Charge transfer excitations (CTE) are of high importance in photovoltaics, organic electronics and molecular and organic magnetism. Range separated funtionals (RSF) can be used to correctly determine the energetics of CTEs within linear response time dependent density functional theory (TDDFT).

TDDFT becomes numerically very demanding on grids if hybrid or RSF are used due to the inclusion of exact exchange derived from Hartree-Fock theory.

We present an implementation of RSF on real space grids and discuss a way to circumvent the problem mentioned above by utilizing Huzinagas improved virtual orbitals (IVOs) that form an improved basis for this type of calculations. The CTE energetics can obtained by means of DFT ground-state calculations using IVOs[1].

[1] R. Würdemann, M. Walter, J. Chem. Theory Comput. 2018, 14, 7, 3667-3676

CPP 12.21 Mon 18:00 P1

Unravelling Superpositions in GI-XPCS by simultaneous GT-GI-XPCS on Spincoated Thin Films — •Christopher R. Greve[1], Meike Kuhn[1], Fabian Eller[1], Guillaume Freychet[3], Alexander Hexemer[2], Lutz Wiegart[3], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]CAMERA, Lawrence Berkeley National Lab Berkeley CA, USA — [3]NSLSII, Brookhaven National Lab, Upton NY, USA

X-Ray Photon Correlation Spectroscopy (XPCS) is a flexible tool to quantify dynamics on the nanometer scale in bulk samples and is used in grazing incidence (GI) geometry for application to thin films. By measurements in GI geometry distortions to the scattering signal are introduced, related to refraction and reflection events, known from the Distorted Wave Born Approximation (DWBA). These reflection and refraction events lead to superpositions of signal on the detector, resulting in alterations of analyzed quantities. We applied an approach to quantify the influence of events within the DWBA on decorrelation analysis by measuring grazing incidence transmission (GT) XPCS and GI-XPCS simultaneously for various thin films. Combining GI-GT-XPCS results with calculations of Fresnel coefficients within the simplified DWBA the origin of scattering contributions is determined. Calculations of the non-linear effect of refractions are added to identify comparable regions within GI and GT. Thus, elucidating differences for phenomena like altered decorrelation times, allowing a valid analysis of GI-XPCS experiments for certain experimental conditions.

CPP 12.22 Mon 18:00 P1

Propagation of learned sequence patterns to larger chain length using TransEncoder neural networks — •Huzaifa Shabbir, Marco Werner, and Jens Uwe Sommer — Leibniz Institute for Polymer Research Dresden

In this work, we investigate artificial neural networks that are capable of learning and transferring hidden variables in chemical sequences from a small sequence length to a larger one. Patterns in the relation between the hydrophilic/hydrophobic sequence of a copolymer and its free energy of interaction with a lipid membrane have been learned with the aid of AutoEncoder neural networks, which were employed to translate between these two properties (TransEncoder)[1]. We demonstrate that the latent space parameters learned by the TransEncoder allow for a physical interpretation of the contributions to the free energy. Furthermore, the learned patterns for a smaller sequence length can be transferred towards a higher sequence length of our interest, which not only significantly reduces the number of training examples required but also increases the accuracy in comparison to the training for individual polymer sequence length. We investigate the computational efficiency and the convergence of learned patterns when multiple chain lengths are addressed at once.

[1] M. Werner, ACS Macro Letters 10, 1333 (2021).

CPP 12.23 Mon 18:00 P1

Crystallization of short polymer chains at hard walls: stochastic approximation Monte Carlo simulation (SAMC) — •Evgeniia Filimonova, Timur Shakirov, and Viktor Ivanov — Martin- Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany

Our research is devoted to crystallization in polymer melts in the presence of hard walls. An interface to a solid material can initiate crystallization in polymer liquids by either heterogeneous nucleation or prefreezing. Our goal is to reveal physical factors which are responsible for one of these two scenarios of surface-induced polymer crystallization. We use coarse-grained model and perform stochastic approximation Monte Carlo (SAMC) simulation. We have developed an approach that allows us to identify the translational and orientational local ordering by means of comparing our system configurations with reference crystalline structures of different symmetries. In addition to calculating the usual order parameters (Steinhardt parameters, common neighbours analysis, nematic order parameter, etc.), we suggested new order parameters based on scalar products of bonds between nearest neighbours. We 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). A change in the crystal structure accompanying a change in density at different energies is also shown. Financial support of the International Graduate School AGRIPOLY supported by the European Social Fund (ESF) and the Federal State Saxony-Anhalt is acknowledged.

CPP 12.24 Mon 18:00 P1

Simulation of reversible chain association using the reaction ensemble Monte Carlo — •Pablo M. Blanco and Peter Košovan — Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 00 Prague 2, Czech Republic.

Reversible association reactions are the key feature of many self-healing polymeric materials and controlled release systems. Simulations and theory are lagging behind the experimental progress in investigating such systems, partly due to the lack of a suitable implementation of an algorithm that would allow for such reversible reactions. In this work, we present an implementation of such reversible reactions within the Reaction-ensemble Monte Carlo framework (RxMC). To validate the algorithm, we simulated the polycondensation reactions, illustrated in Fig.1 (top). These reactions are common in polymer chemistry, and analytical predictions of the distribution of chain lengths at equilibrium are available, serving as an ideal test case for numerical simulations. Starting from the free monomers, we let the system evolve towards equilibrium, resulting in an ensemble of chains of various chain lengths, depending on the value of the equilibrium constant of the reaction. By comparing our simulation results with the theoretical predictions, we investigate the limitations of the algorithm, possible finite-size effect, and efficiency of its implementation. After initial validation, this reaction algorithm will be implemented in the ESPResSo simulation software (www.espressomd.org) that will enable its application to a broad class of problems involving reversible association reactions.

CPP 12.25 Mon 18:00 P1

Modelling electrode interfaces via multi-scale simulations — •Henrik Konstantin Jäger, Philipp Stärk, and Alexander Schlaich — Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Germany

We investigate the interactions of ions at a graphene interface via first-principle simulations using ab initio molecular dynamics. In a multi-scale approach we employ first principle calculations to parametrize semi-classical electrode models based on the Tomas-Fermi screening approach, allowing to access dynamics and adsorption at common electrode-electrolyte interfaces.

CPP 12.26 Mon 18:00 P1

Combined first-principles statistical mechanics approach to sulfur structure in organic cathode hosts for polymer based lithium-sulfur (Li-S) batteries — •Yannik Schütze[1,2], Ranielle Oliveira de Silva[1,3], Jiaoyi Ning[1], Jörg Rappich[1], Yan Lu[1,3], Victor G. Ruiz[1], Annika Bande[3], and Joachim Dzubiella[1,4] — [1]Helmholtz-Zentrum Berlin für Energie und Materialien GmbH, Germany — [2]Freie Universität Berlin, Germany — [3]Universität Potsdam, Germany — [4]Albert-Ludwigs-Universität Freiburg, Germany

Polymer-based batteries that utilize organic electrode materials are considered viable candidates to overcome the common drawbacks of lithium-sulfur (Li-S) batteries. A promising cathode can be developed using a conductive, flexible, and free-standing polymer, poly(4-thiophen-3-yl)benzenethiol) (PTBT), as the sulfur host material. Here, we present a combination of electronic structure theory and statistical mechanics to characterize the structure of the initial state of the charged cathode on an atomic level. We perform a stability analysis of differently sulfurized TBT dimers as the basic polymer unit calculated within density-functional theory (DFT) and combine this with a statistical binding model for the binding probability distributions of the vulcanization process. This multi-scale approach allows us to bridge the gap between the local description of the covalent bonding process and the derivation of the macroscopic properties of the cathode.

CPP 12.27 Mon 18:00 P1

Correcting Coarse-Grained Dynamics of Molecular Liquids and Their Mixtures Using an Efficient Iterative Memory Reconstruction Method — •Madhusmita Tripathy, Viktor Klippenstein, and Nico FA van der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Generalized Langevin equation (GLE) based coarse-grained (CG) models are considered to be the most reliable models for dynamically consistent coarse-graining [1]. However, their implementation in molecular simulation is not straight-forward owing to their inherent complexity [2]. With an aim to employ computationally tractable GLE based CG models for dynamic coarse graining of complex molecular systems, we coarse-grain two molecular liquids and their mixtures at various compositions following a novel iterative optimization scheme. Using the memory kernel from an isotropic GLE model as a starting point, we use an efficient iterative memory reconstruction method, which can closely reproduce the underlying fine-grained (FG) dynamics, assessed in terms of the velocity auto-correlation function, within a few iterations. We use this iterative method to correct the artificial dynamic speed-up in CG molecular dynamics (MD) simulations of pure molecular liquids and the relative dynamic speed-up in their mixtures. Furthermore, we investigate the transferability of the resulting memory kernels to molecular mixtures with varying composition.

[1] Klippenstein et al. J. Phys. Chem. B 125 (19), 4931-4954 [2] Glatzel and Schilling, Europhys Lett. 136 36001 (2021)

CPP 12.28 Mon 18:00 P1

Aggregation of flexible-semiflexible multiblock-copolymers in a dilute solution: MD simulation — •Viktor Ivanov[1,2], Elizaveta Sidler[2], Julia Martemyanova[2], Timur Shakirov[1], and Wolfgang Paul[1] — [1]Martin-Luther-University Halle-Wittenberg, Institute of Physics, 06099, Halle, Germany — [2]Moscow, Russia

We study aggregation of several regular multi-block copolymer chains in a dilute solution. Chains consist of flexible (F) and semi-flexible (S) blocks with equal composition of F- and S-units having different affinity to a solvent, which is poor for both components. We use coarse-grained MD simulation. Our main goal is to find conditions (values of model parameters) for a shape-persistent aggregation of globules with different non-trivial globular morphologies which are formed in poor solvent, including structures with high orientational ordering of S-blocks and with micro-segregation of S- and F-blocks. Stable aggregates of the following highly anisotropic morphologies have been obtained: "core-shell", "bundle", "dumbbell", "disk", worm-like micelles ("tubes"). The driving forces for formation of structured globules and their anisotropic aggregates are usual van-der-Walls interactions, block length and intramolecular stiffness (there are no specific interactions in our model). 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 computational resources.

CPP 12.29 Mon 18:00 P1

A combined experimental-theoretical study of azo-SAM restructuring under light stimulus: New insights — Alexey Kopyshev[1,2], Amrita Pal[1], Svetlana Santer[2], and •Olga Guskova[1] — [1]IPF Dresden, 01069 Dresden, Germany — [2]University of Potsdam, 14469 Potsdam, Germany

The topography transformation of the self-assembled (SAM) layers of azobenzene (azo) surfactant [1] on mica is studied using AFM and modeled in all-atom MD simulations. Under blue light, when azo adopts the trans-state, the smooth SAMs are formed. Under UV stimulus due to a shift in equilibrium between trans and cis isomers, a rapid change in the topography of SAMs occurs. Subsequent blue light irradiation leads to the stabilization of SAMs and smoothing of the upper layers. The explanation of the layer restructuring/mass transport is proposed in simulations. First, we observe that the cis isomers diffuse slower within the adsorbed layers. Second, the expulsion of the cis isomers from SAM is detected independently of the layer compositions. Third, the vertical diffusion for trans isomers is negligible, whereas for cis-state it is comparable to diffusion within the layer. Thus, the change in the topography of SAMs under UV light seen in AFM is related to the vertical diffusion of cis azo. The work is supported by DFG (project GU1510/5-1). [1] Titov E. et al. ChemPhotoChem 5 (2021) 926.

CPP 12.30 Mon 18:00 P1

Molecular switch based on bithiophene-azobenzene: How to control conductance through the monolayer using light — •Vladyslav Savchenko and Olga Guskova — IPF Dresden, 01069 Dresden, Germany

Molecular switches based on azobenzene (azo) are defined as light-responsive molecules which can change between two configurational states. Responsive azo monolayers can be used to modulate the work function of the electrodes. In this study, we investigate using DFT what happens to the structures, electronic properties, and the charge redistribution within azo-bithiophene (azo-bt) monolayers depending on the light stimulus. Two types of switches differing in the order of azo and bt counting from the anchor group are modeled: azo-bt and bt-azo. Bt-azo switch is known from the literature [1], while the azo-bt is a product of rational design [2]. We study trans- and cis-isomers for each switch being in a contact with a gold cluster (C-AFM tip). A giant ON/OFF conductance ratio upon UV light observed in the experiment [1] results from an improved electronic coupling between the cis-isomers and the gold tip (ON-state) [1]. The trans-isomers of the simulated switches play the role of the insulators (OFF-state). Moreover, we show which molecular properties are enhanced by molecular design. This study opens up new avenues for the development of the rational design of electrode surface modifications. The work is supported by DFG, project GU1510/5-1. [1] Smaali K. et al. ACS Nano 4 (2021) 2411. [2] Savchenko V.A. et al. Herald of TvSU. Ser. Chemistry 3 (2021) 7.

CPP 12.31 Mon 18:00 P1

Non-invasively induced amphiphilic self-assemblies from orthogonally switchable block copolymers — •Peiran Zhang[1], René Steinbrecher[2], Andre Laschewsky[2,3], Peter Müller-Buschbaum[4], and Christine M. Papadakis[1] — [1]Fachgebiet Physik weicher Materie, Physik-Department, TU München, Garching — [2]Institut für Chemie, Universität Potsdam — [3]Fraunhofer IAP, Potsdam-Golm — [4]Lehrstuhl für Funktionelle Materialien, Physik-Department, TU München, Garching

Amphiphilic self-assemblies arising from orthogonally switchable block copolymers are promising candidate in drug delivery, due to their structure and transformation diversity, which is superior to the presently most studied singly responsive copolymers [1]. To induce this process completely non-invasively, light in combination with temperature is utilized as the stimulus. Introduction of suitable photoactive functional groups could modulate the LCST of the copolymer, thereby achieving the stage that all aggregate scenarios could be concluded in a certain temperature range. For characterization of the copolymer structure, measurements are implemented by dynamic light scattering (DLS), small angle X-ray scattering (SAXS) and -neutron scattering (SANS), while the phase behavior as well as phase transition kinetics are investigated by the time-resolved scattering methods.

[1] C. M. Papadakis, et al., Langmuir 2019, 35, 9660-9676.

CPP 12.32 Mon 18:00 P1

Effect of architecture in thermoresponsive methacrylate terpolymers based on PEG analogues — •Feifei Zheng[1], Eirini Melampianaki[1], Wenqi Xu[1], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]Physics Department, Technical University of Munich, Garching, Germany — [2]Department of Materials, Imperial College, London, England

The LCST polymers have attracted great interest for the biomedical sectors, as they have the advantage of being water-soluble at room temperature, while they can form a gel at body temperature [1]. Here, we address the effect of polymer architecture of poly(ethylene glycol) based thermoresponsive terpolymers featuring A, B and C blocks. These consist of the hydrophilic oligo(ethylene glycol) methyl ether methacrylate (OEGMA300, A), hydrophobic n-butyl methacrylate (B), and thermoresponsive di(ethylene glycol) methyl ether methacrylate (C). Several architectures have been synthesised via group transfer polymerisation, varying from statistical, to gradient to block structures. The results from dynamic light scattering indicate that the BABC tetrablock terpolymer and ABC gradient polymer form smaller micelles than ABC triblock terpolymer. This difference points to the importance of the exposed OEGMA300 block for micelle stabilization: bending it back in the BABC architecture enhances the effect of the thermoresponsive block on the thermal behavior.

[1] A. P. Constantinou, B. Zhan et al., Macromolecules, 2021, 54, 1943.

CPP 12.33 Mon 18:00 P1

Unique colorimetric response of polydiacetylene-Na^+ microcrystals for detection of hydrochloric acid by naked eye — •Rungarune Saymung[1], Christine M. Papadakis[2], Nisanart Traiphol[3], and Rakchart Traiphol[1] — [1]School of Materials Science and Innovation, Faculty of Science, Mahidol University, Nakhon Pathom, Thailand — [2]Physics Department, Technical University of Munich, Garching, Germany — [3]Materials Science Department, Faculty of Science, Chulalongkorn University, Bangkok, Thailand

Polydiacetylenes (PDA), a class of conjugated polymers, are very promising as colorimetric sensors because the change of the color can be easily observed. The commercially available PDA with carboxylic head groups changes color from blue at acidic to red in basic condition. To develop this class of materials for pH sensing applications, many research groups synthesize PDA-based materials by structural modification or addition of foreign materials. Studies by our research group illustrate that incorporating ZnO nanoparticles with PDAs lead to colorimetric response to both acids and bases. Herein, we explore a new route by introducing Na^+ ions into the PDA system. Upon exposure to hydrochloric acid (HCl) solution, the PDA-Na microcrystals exhibit a unique red to blue color-transition, which has never been observed before. To understand the origins of this behavior, various techniques are employed including Fourier-transformed infrared spectroscopy (FT-IR), scanning electron microscope (SEM), and X-ray diffraction (XRD).

CPP 12.34 Mon 18:00 P1

Anionic surfactant detection using polydiacetylene-based nanocomposites — •Watsapon Yimkaew[1], Christine M. Papadakis[2], Rakchart Traiphol[3], and Nisanart Traiphol[1] — [1]Laboratory of Advanced Chromic Materials, Department of Materials Science, Faculty of Science, Chulalongkorn University, Bangkok, Thailand — [2]Physics Department, Technical University of Munich, Garching, Germany — [3]Laboratory of Advanced Polymer and Nanomaterials, School of Materials Science and Innovation, Faculty of Science, Mahidol University, Nakhon Pathom, Thailand

Polydiacetylenes (PDAs) are color-responsive polymers to various stimuli. The development of PDAs as anionic surfactant sensors by structural modification involved complicated and costly processes. In this study, we introduce a facile approach for preparing polydiacetylene/zinc (II) ion/zinc oxide (PDA/Zn2+/ZnO) nanocomposites utilized for anionic surfactant detection. Cationic surfactant, cetyltrimethylammonium bromide (CTAB) is incorporated into the nanocomposites via a simple mixing process to adjust their color transition behaviors. Addition of CTAB at 1 mM induces the blue-to-yellow color transition of the nanocomposites. Interestingly, the nanocomposites exhibit yellow-to-red color transition in response to sodium dodecyl sulfate (SDS). This demonstrates the ability of the nanocomposites as anionic surfactant sensors. A key mechanism of the color transition is the interaction between CTAB and SDS, which induces perturbation in the outer layers of the nanocomposites.

CPP 12.35 Mon 18:00 P1

Tunable morphologies in charged multiblock terpolymers in thin film geometry: effect of solvent vapor annealing — •Bahar Yazdanshenas[1], Florian A. Jung[1], Maximilian Schart[1], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]Technische Universität München, Physik-Department, Fachgebiet Physik weicher Materie, Garching, Germany — [2]University of Patras, Department of Chemical Engineering, Patras, Greece

Thin films of a pentablock terpolymer with a symmetric architecture of two types of pH-responsive midblocks and short hydrophobic end blocks are investigated. As-prepared spin-coated films from different pH-values have previously shown highly tunable and non-monotonous behavior of the lateral structure sizes, based on the charge [1]. However, with the high glass transition temperatures of the middle pH-responsive block and the hydrophobic end blocks, the films were not necessarily in equilibrium. Here, we investigate further accessible morphologies by swelling the films in the vapors of solvents having different selectivity. Results from spectral reflectance and atomic force microscopy suggest that water (exclusively swelling the pH-responsive blocks) leaves the nanostructures intact, while methanol (swelling all blocks) results in a reorganization. Mixtures of these vapors allow to tune the solubilities of the blocks and thus to find the minimum amount of methanol needed for equilibration.

[1] F. A. Jung, C. M. Papadakis et al., Adv. Funct. Mater. 2021, 31, 2102905.

CPP 12.36 Mon 18:00 P1

Transport of thin water films: from thermally activated random walks to hydrodynamics — Simon Gravelle[1], Christian Holm[1], and •Alexander Schlaich[2] — [1]Institute for Computational Physics, University of Stuttgart, Germany — [2]Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Germany

Under ambient atmospheric conditions, a thin film of water wets many solid surfaces, including insulators, ice, and salt. The film thickness as well as its transport behavior sensitively depend on the surrounding humidity. Understanding this intricate interplay is of highest relevance for water transport through porous media, particularly in the context of soil salinization induced by evaporation. Here, we use molecular simulations to evaluate the transport properties of thin water films on prototypical salt and soil interfaces.

Our results show two distinct regimes for water transport: at low water coverage, the film permeance scales linearly with the adsorbed amount, in agreement with the activated random walk model. Finally, in the context of water transport through porous material, we determine the humidity-dependent crossover between a vapor dominated and a thin film dominated transport regimes depending on the pore size.

CPP 12.37 Mon 18:00 P1

Predicting static wetting morphology of aqueous drops on lubricated surface — •Shivam Gupta, Bidisha Bhatt, Meenaxi Sharma, and Krishnacharya Khare — Indian Institute of Technology Kanpur, Kanpur, India

Static wetting behavior of liquid drops on thin liquid-coated solid surfaces is very different compared to dry solid surfaces. Conventionally, the equilibrium wetting behavior on deformable (soft or thin liquid coated) surfaces is characterized by the Neumann's contact angle, which solely depends on the various interfacial energies of the participating phases. However, due to the difficulty in identifying the Neumann's point, it is often convenient to define apparent contact angles on such surfaces. By controlling the various interfacial energies, drops can be either made to directly contact the substrate or float on the thin liquid layer supported by the substrate resulting in different apparent angles and thus different wetting morphology. Although such systems are highly prevalent, however, to our knowledge, there is no study reported to date that can beforehand predict the static wetting behavior and the quasi-static interfacial profiles as a function of various system parameters, e.g., substrate wettability, thickness of the liquid film, and drop volume. We propose a method to beforehand predict the interfacial profiles using numerical computation with Surface Evolver software. Experimental studies are also performed to validate the simulations. A good quantitative agreement is found for the variation of the drop contact angle as a function of various systems parameters.

CPP 12.38 Mon 18:00 P1

In-situ white light, near infrared spectroscopy on thin films and photonic crystals of nanoporous silicon during liquid imbibition — •Guido Dittrich[1,2], Raul Urteaga[3], and Patrick Huber[1,2] — [1]Hamburg University of Technology, Institute of Materials and X-Ray Physics, 21073 Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Centre for X-Ray and Nano Science CXNS, Hamburg, Germany — [3]IFIS-Litoral (Universidad Nacional del Litoral-CONICET), Guemes 3450, 3000 Santa Fe, Argentina

Nanoporous materials offer a high specific surface area and spatial confinement. Scientists are aiming to abuse these properties for functional materials in a variety of fields, e.g. thermoelectrics, catalysis, Lab-on-a-Chip as well as energy storage and harvesting applications. Understanding the fundamental transport mechanisms on the nanoscale is required and drives the progress. We present a method to measure liquid imbibition in nanoporous silicon (np-Si) with a resolution even resolving spreading of ultra-thin precursor films in nanopore space with a time resolution of microseconds. Therefore, a photonic crystal (PC) is etched in at a chosen height during the fabrication. The PC has a specific resonance wavelength, which can be monitored with white light spectroscopy. Imbibition by fluids, in our case oligostyrenes, into the central defect of the PC changes the effective refractive index and causes a proportional shift of the resonance wavelength. This offers very localized information on the nanopore filling at the position of the PC. Producing only thin np-Si films, one can measure the shift of the thin film interference with a NIR-spectrometer simultaneously.

CPP 12.39 Mon 18:00 P1

Single-nanochannel X-ray diffraction on the liquid crystal C8BTBT confined in anodic aluminium oxide membranes — •Mark Busch[1,2], Zhuoqing Li[1,2], Milena Lippmann[2], Andreas Schropp[2], Johannes Hagemann[2], Christian Schroer[2,3], and Patrick Huber[1,2] — [1]TU Hamburg, Institut für Material- und Röntgenphysik — [2]Deutsches Elektronen-Synchrotron DESY — [3]Universität Hamburg

We investigate the self-assembly of the liquid crystal C8BTBT within anodic aluminium oxide (AAO) nanochannels in dependence of channel wall chemistry and the diameter of the channels from 60 to 180 nm. Conventional X-ray diffraction experiments use a comparatively large beam and therefore deliver a structural information which is averaged over a large number of nanochannels. In contrast here we investigate the structure of liquid crystals within individual nanochannels by employing an X-ray beam with a diameter in the nanometre range.

CPP 12.40 Mon 18:00 P1

Investigation of the charge transport of ionic liquid post-treated PEDOT:PSS thin films with in-situ surface plane impedance spectroscopy, under the influence of varying temperature and humidity — •Tobias Schöner[1], Anna Lena Oechsle[1], and Peter Müller-Buschbaum[1,2] — [1]Lehrstuhl für

Funktionelle Materialien, Physik- Department, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

Thermoelectric materials based on polymers are attractive due to their large-scale and low cost processability, high mechanical flexibility, low or no toxicity, lightness and intrinsically low thermal conductivity. One highly investigated polymer with promising thermoelectric properties is poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS). The post-treatment of PEDOT:PSS thin films with ionic liquids (ILs) enhances the thermoelectric properties for the practical application by simultaneously improving the inter-domain conductivity and optimizing the charge carrier concentration. Our recent investigation focuses on the influence of the environmental parameters temperature and humidity on the electronic and ionic charge transport properties in the thin films. For this, the thermoelectric films are contacted with a self-built setup in a planar way and inserted into a humidity chamber. By using a potentiostat surface-plane Galvanostatic Electrochemical Impedance Spectroscopy (GEIS) measurements under alternating humidity and temperature can be performed.

CPP 12.41 Mon 18:00 P1

Optimization Strategies for Purely Organic Room-Temperature Phosphorescence — •Heidi Thomas and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, TU Dresden

The development of organic materials displaying room-temperature phosphorescence (RTP) with lifetimes in the range of several hundred milliseconds is a research field that has attracted more and more attention in the last years. By using amorphous purely organic systems, we have been able, for example, to develop programmable luminescent tags. Still, the potential of such emitter systems is far from being exploited. We present a new family of organic luminescent derivatives embedded in amorphous matrices with phosphorescence lifetimes up to 2.6 s, extending their applicability. Hydrogen bonds between the emitters and the matrix presumably suppress vibrational dissipation, thus enabling bright long-lived phosphorescence. Further optimization of the host:emitter system is related to the film preparation technique. By varying host polymer, post-annealing temperature, and fabrication procedure, we analyze the phosphorescent lifetime, the photoluminescent quantum yield, and the phosphorescence-to-luminescence ratio. The film thickness turns out to affect the performance the most: Going from thin to thick spin-coated films, the phosphorescence lifetime could be increased by a factor of up to 2.5.

CPP 12.42 Mon 18:00 P1

Investigating the Impact of Surfactants on Perovskite Crystallization during Thin Film Solution Processing Using In Situ Optical Spectroscopy — •Tobias Siegert, Simon Biberger, Konstantin Schötz, and Fabian Panzer — University, Bayreuth, Germany

Recent reports have shown that adding surfactants in the solution processing of halide perovskites, e.g. by blade-coating, can improve their morphology and optoelectronic properties[1]. In general the crystallization processes of halide perovskites that occur during thin film formation largely determine the final film morphology. Thus, here we investigate the change in crystallization dynamics upon addition of surfactants to the solution processing of halide perovskites. We monitor the film formation processes by multimodal optical in situ spectroscopy[2], so that detailed insights about the film formation process of halide perovskites can be gained[3,4]. This finally allows us to elucidate the exact role and the impact of the presence of surfactants during solution processing on the crystallization behavior of the perovskite.

[1] Deng et al. Nat Energy 2018
[2] Buchhorn, Wedler, Panzer. J. Phys. Chem. A 2018
[3] Chauhan, Zhong et al. J. Mater. Chem. A. 2020
[4] Schötz et al. Adv. Optical Mater. 2021

CPP 12.43 Mon 18:00 P1

Fabrication and Characterisation of Two-Step Slot-Die Coated Methylammonium-Formamidinium Lead Iodide Perovskite Solar Cells — •Thomas Baier, Manuel A. Reus, Lennart K. Reb, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Perovskite solar cells (PSCs) are very promising in contributing in the renewable energy mix of the future. They have high power conversion efficiencies and are made of low-cost materials. Especially in combination with slot-die coating as promising thin-film deposition technique for organic-inorganic hybrid perovskite materials, they offer the chance for fast and cheap roll-to-roll solar cell production.

In this work two-step slot-die coated lead iodide layers and slot-die coated methylammonium-formamidinium iodide perovskite solar cells have been prepared. Depending on slot-die coating parameters and additives used in the ink that enhance thin-film formation and optoelectronic properties of the final perovskite semiconductor absorber, morphology changes are observed in the final film. The morphology is investigated by reciprocal (X-ray diffraction) and real-space methods (SEM). Furthermore, the two-step slot-die coated solar cells are produced and characterized via their respective performance parameters.

CPP 12.44 Mon 18:00 P1

First-principles study of the electronic and optical properties of perovskite solution precursors — •Freerk Schütt[1], Ana M. Valencia[1,2], and Caterina Cocchi[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Humboldt-Universität zu Berlin und IRIS Adlershof, Berlin

Metal halide perovskites have shown great promise for next-generation opto-electronic applications but the predominant employment of Pb poses a problem in terms of environmental sustainability of these compounds. Replacing Pb with Sn represents a viable solution, however, despite recent efforts in this direction [1], knowledge of Sn-based perovskites and precursors is to date still insufficient. In a first-principles work based on time-dependent density-functional theory coupled to the polarizable continuum model, we systematically investigate electronic and optical properties of SnI_2M_4 complexes, with M being common solvent molecules. We find that the structural, electronic, and optical properties are strongly affected by the choice of the solvent. By rationalising the behavior of 15 of such compounds even in comparison with lead-halide counterparts [2,3], we provide useful indications to complement experiments in the choice of the solvent molecules for SnI_2-based solution complexes and in their characterization towards the production of thin films. [1] Di Girolamo et al., ACS Energy Lett. 6, 959 (2021). [2] Schier et al., Phys. Status Sol. B 258, 2100359 (2021). [3] Procida et al., PCCP 23, 21087 (2021).

CPP 12.45 Mon 18:00 P1

Ionic liquids tailoring crystal orientation for stable and high fill factor perovskite solar cells — •Yuqin Zou[1], Lukas V Spanier[1], Julian E Heger[1], Shanshan Yin[1], Christopher R Everett[1], and Peter Müller-Buschbaum Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

Ionic liquids with superior electrical conductivity and thermal stability are used as effective and practical dopants to improve the long-term operation stability and the photovoltaic performance of perovskite solar cells (PSCs). We study different ionic liquids in the perovskite component. Using grazing-incidence wide-angle X-ray scattering (GIWAXS), we discover that the incorporation of ionic liquids is beneficial for obtaining homogeneous spherical nano-particle films and tuning the film crystal orientation. We select 1-butyl-1-methylpyrrolidinium tetrafluoroborate (Pyr13BF4) as the main additive to investigate the charge carrier dynamic behavior of PSCs underdoped with Pyr13BF4 using TRPL, TPC, TPV and OCVD methods. In addition to enhancing the fill factor and optimizing energy level alignment, this additive promotes charge transfer and extraction, reduces the charge carrier accumulation in the bulk, and retards recombination. Under ambient atmosphere, the un-encapsulated PSCs retain 97% of their initial efficiencies for 4368 h.

CPP 12.46 Mon 18:00 P1

Improving morphology and efficiency of slot-die coated perovskite solar cells — •Christoph G. Lindenmeir[1], Andrea Vitaloni[1], Lennart K. Reb[1], Manuel A. Reus[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

During the last years perovskite solar cells (PSCs) received high attention in industry and research for sustainable power production. Especially due to their low material costs, low weight, high power conversion efficiencies, and the possibility to fabricate them via simple solution-based deposition techniques like slot-die coating or spray coating. Because of the possibility of up-scaling and using minimal material, slot-die coating is one of the most promising techniques to produce high efficiency PSCs. In this work, we compare the properties of slot-die coated PSCs with different perovskite compositions. The perovskite layer is printed out of a solution, containing different ratios of lead iodide (PbI2), methylammonium iodide (MAI), formamidinium iodide (FAI), and methylammonium chloride (MACl) in a solvent mixture of 2-methoxyethanol (2-ME) and dimethyl sulfoxide (DMSO). To improve the film quality of the printed perovskite layer, the influence of nitrogen gas quenching is extensively studied and the print process optimized. The resulting high-quality thin films are analyzed with optical and structure characterization methods like spectroscopy and X-ray scattering methods. For further information, current-voltage and external quantum efficiency measurements are carried out.

CPP 12.47 Mon 18:00 P1

Slot-die coated perovskite quantum dot layers for solar cell application — •Ahmed Krifa[1], Manuel A. Reus[1], Lennart K. Reb[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

Perovskite quantum dots (PQDs) are semiconductor nanocrystals that have received tremendous attention in photovoltaic devices due to their exceptional optical and electronic properties. PQD solar cells (PQDSCs) have shown great potential to overcome many drawbacks of their large-grain perovskite thin-film (often called bulk) counterparts, such as high defect tolerance and better stability due to the controlled surface properties of the quantum dots. Over the past few years, PQDSCs have shown a quick increase in efficiency, already exceeding 16%, and high stability. However, the fabrication of these solar cells is based on the spin-coating technique, which leads to significant waste. In this work, we develop and optimize a printing process for PQDs layers and study them with various techniques such as UV-Vis, scanning electron microscopy and X-ray diffraction to achieve an up scalable fabrication of PQDSCs.

CPP 12.48 Mon 18:00 P1

In situ study of supperlattice self-assembly during printing of perovskite quantum dot films for solar cell applications — •David P. Kosbahn[1], Manuel A. Reus[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

Research into quantum dots (QDs) of lead halide perovskites (LHPs) has become increasingly popular due to their stability and tunable optoelectronic properties. Their controllable surface chemistry and simple preparation make them a promising alternative to bulk perovskite solar cells. The power conversion efficiency (PCE) of $Cs_xFA_{1-x}PbI_3$ QD solar cells (QDSCs) has been steadily rising, up to a recent record efficiency surpassing 16%. However, the orientation and self-assembly of the colloidal precursor into a superstructure is not yet well-understood. In this work, we study the formation of perovskite QD films using in situ grazing-incidence wide-angle X-ray scattering (GIWAXS) in real time, to achieve a better understanding of the kinetics involved in their fabrication.

CPP 12.49 Mon 18:00 P1

Operando study of light and moisture induced degradation of perovskite solar cell — •Kun Sun[1], Julian E. Heger[1], Manuel A. Reus[1], Xinyu Jiang[1], Lukas V. Spanier[1], Sigrid Bernstorff[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Elettra-Sincrotrone Trieste, 34149 Basovizza — [3]MLZ, TU München, 85748 Garching

Perovskite solar cells (PSCs) are among the most promising photovoltaic technologies and reached a certified 25.5% efficiency owing to their tuneable bandgap, high charge 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 and solar cell performance under 1-sun illumination and high humidity. We find that PSCs fabricated with and without caesium iodide (CsI) show differences in the device degradation and morphology change. 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, 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 12.50 Mon 18:00 P1

Non-invasive characterization of degradation in inverted planar perovskite solar cells via reflectance and optical modelling. — •Chikezie Williams Ugokwe[1,2], Kehinde Ogunmoye[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [2]Institute for Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

Despite gains in efficiency since their discovery a little more than a decade ago, hybrid perovskite solar cells (PSCs) are still plagued by poor stability. This poor stability also interferes with their characterization to the point where widely used and easily applicable methods of studying in situ degradation, such as scanning electron microscopy, X-ray diffraction, impact the result because they are invasive and introduce some forms of degradation themselves.

We pursued a non-invasive approach for characterizing the evolution of degradation in PSCs using a combination of optical characterization, modelling, and simulation. Using a software package for coherent light propagation in thin film layer stacks, reflectance and transmittance spectra were used to model the complex refractive index of each functional layer. The evolution of degradation was then studied for ageing methylammonium PSC using periodically measured reflectance data. We will discuss if the evolution of lead iodide, the undoubtable by-product of degradation can be detected using optical simulation.

CPP 12.51 Mon 18:00 P1

Charge Carrier Properties of $Cs_2AgBiBr_6$ in Thin Films for Perovskite Solar Cells — •Tim P. Schneider, Jonas Horn, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

The double perovskite $Cs_2AgBiBr_6$ is regarded as a potential candidate to replace the toxic lead perovskites currently used in perovskite solar cells and can potentially be used for photo- and x-ray detection. For any such technical application the electrical properties of the double perovskite play an important role. Therefore, the charge transport in $Cs_2AgBiBr_6$ was systematically studied in different sample geometries. Thin films were prepared onto micro-structured interdigitated metal electrode arrays as well as sandwiched between different electron-conducting or hole-conducting layers that are often used in perovskite solar cells, to achieve single-carrier-devices. Aside from estimates of the conductivity and a discussion of possible trapping of charge carriers, the obtained current-voltage characteristics yielded insights into contact formation, hysteresis and intrinsic ion migration. Further, atomic force microscopy showed a strong influence of the underlying substrate on the morphology of the $Cs_2AgBiBr_6$ thin films.

CPP 12.52 Mon 18:00 P1

Decoding the Self-assembled Plasmonic Nano-structure in Colloidal Quantum Dots for Photodetectors — •Tianfu Guan, Wei Chen, Christian L. Weindl, Suzhe Liang, and Peter Müller-Buschbaum — Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85748 Garching, Germany

Hybrid plasmonic nanostructures have raised great interest for being used in a variety of optoelectronic devices, due to the surface plasmon resonance (SPR). Charge carriers trapped in colloidal quantum dots (QDs) at localized surface defects is a key issue in photodetectors. Self-assembled hybrid metal/quantum dots can couple plasmonics and quantum properties to photodetectors and modify their functionality. Arranged and localized hybrid nanostructures impact on excitons traps and light harvesting. Here, we demonstrate a coupling hybrid structure using self-assembled gold nanoparticles (Au NPs) doped in PbS QDs solid for mapping the interface structures and the motion of excitons. Grazing incidence small angle X-ray scattering (GISAXS) was used to characterize the order of the Au NPs in the hybrid structure. Furthermore, by correlating the sizes of the Au NPs in the hybrid structure with corresponding differences in photodetector performance, we could obtain the interface carriers trapping influences in the coupling structure.

CPP 12.53 Mon 18:00 P1

Einfluss von CO2 auf die Zusammensetzung von Produkten bei der Hydrierung von Kohlenstoffoxiden an einem Katalysator mit GdFeO3-Perowskitstruktur — •Polina Akhmina — Moscow, Russia

Heute stehen viele Menschen in der Welt vor der Notwendigkeit, den ständig wachsenden Energiebedarf zu decken. Einen wichtigen Platz nimmt die Energie von Kohlenwasserstoffen ein, eine der vielversprechenden Methoden zu deren Synthese ist die Fischer-Tropsch-Synthese. Bakannte Katalysatoren für die Fischer-Tropsch-Synthese sind Verbindungen auf Eisen- und Kobaltbasis, auch komplexe Oxide mit der ABO3-Perowskitstruktur (A-Kation eines Alkali- oder Seltenerdmetalls, B - Übergangsmetallkation) finden ihre Anwendung. Es wurde ein Experiment mit der Feststellung der Wirkung der Einführung von Kohlendioxid in die Zusammensetzung des Synthesegases CO:H2 durchgeführt. Das Reaktionsgemisch wurde auf einem Gaschromatographen mit einer Edelstahlsäule analysiert, die Menge der Produkten wurde aus der Fläche der chromatographischen Peaks bestimmt. Als Ergebnis wurde erfahren, dass, im Fall wenn der Gehalt von CO2 in der Reaktionsmischung 17 % ist (Verhältnis der Reagenzien (CO:CO2): H2 = (1:1:2)), im Vergleich zu der Reaktionsmischung ohne Kohlendioxid, ist eine Erhöhung der Menge der gebildeten leichten Olefinen und eine Erhöhung der Olefin/Paraffin-Verhältnisse bemerkt. Außerdem gab es eine Verringerung der Umwandlung von CO. Einer der möglichen Gründe für die Verringerung der Umwandlung ist das Auftreten eines Boudouard Nebenreaktion: 2CO = C + CO2

CPP 12.54 Mon 18:00 P1

Semiconducting Carbon Nitride Thin Films — •Hsu Thazin Myint[1], Lennart K. Reb[1], Manuel A. Reus[1], Narendra Chaulagain[2], Karthik Shankar[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]University of Alberta, Department of Electrical and Computer Engineering, Edmonton, AB T6G 1H9, Canada — [3]MLZ, TU München, 85748 Garching

Researchers endeavoring for a clean energy resource have focused on a semiconducting material called graphitic carbon nitride (g-C_3N_4). The unique property of this material is being environmentally benign due to its metal-free nature, and high solubility in water. Moreover, the earth-abundance of carbon and nitrogen enables easy synthesis at low costs. The astonishing optoelectronic properties, high stability, and absorption in UV-visible region with band-gap energy of 2.7eV render g-C_3N_4 a prime center for the extensive applications such as solar energy utilization. Fabrication of homogeneous g-C_3N_4 thin films with tailored thickness and morphology is important to develop novel applications. However, the material deposition to achieve homogeneous thin films is still challenging, rendering information about the bulk material properties essential for device application largely unknown to date. In this work, the low waste and scalable slot-die coating method is finetuned to get uniform and high-quality films with good adhesion onto the substrates. The final optimized thin-film properties are studied in terms of spectroscopic, morphological and structural characterization methods.

CPP 12.55 Mon 18:00 P1

Comparison of exciton diffusion in organic and inorganic semiconductors — •Dominik Muth, Marina Gerhard, Gregor Witte, Daniel Bischof, and Sebastian Anhäuser — Philipps Universität, Marburg, Deutschland

The mechanisms of exciton and charge carrier transport in organic and inorganic semiconductors differs greatly. To characterize transport processes on the picosecond time scale, a streak camera coupled with a megahertz laser system is employed. The spatio-temporal evolution of the excitation profile is studied at temperatures between 77 K and 295 K. Detailed analysis of the spatial broadening allows us to estimate the underlying exciton diffusion coefficients as a function of time and temperature. In single crystalline tetracene we find evidence for highly dispersive exciton transport, which indicates that excitons populate more localized states on a time scale of a few hundred picoseconds. Moreover, the diffusion coefficients show clear temperature dependence, which will be discussed in this contribution.

CPP 12.56 Mon 18:00 P1

Matrix Influence on the Photodynamics of a TADF-Emitting Molecule — •Björn Ewald[1], Ulrich Mueller[1], Jonas Gehrig[1], Jonas Bellmann[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The singlet-triplet dynamics of thermally activated delayed fluorescence (TADF) emitters is of high technological relevance for their application in 3rd generation Organic Light Emitting Diodes. In this respect, the molecular and solid-state properties of the matrix material hosting the molecular TADF-dopant, may drastically influence its confirmation, the related energetics and thus, its rate dynamics and the overall OLED efficiency. By virtue of their dark and long-living nature, spectroscopic access to the population dynamics of involved triplet states in such host-guest systems is not trivial. Here we applied a spectroscopic method, based on transient intensity-modulated photoluminescence (TIM-PL). Resting on a generic three level scheme, this technique yields access to the singlet-triplet population dynamics and the corresponding rates in TADF host-guest blends. We studied the photophysics of the TADF-emitter TXO-TPA doped into matrices with different crystalline order (PMMA and mCP). We can confirm that local matrix effects impose a significant impact on the rate dynamics and the singlet-triplet conversion. Particularly the intersystemcrossing rate can be drastically influenced by the local matrix environment. Hence the data obtained by the TIM-PL method, allow for a more rational selection of suited TADF guest-matrix combinations.

CPP 12.57 Mon 18:00 P1

Optically Detected Magnetic Resonance (ODMR) studies on Pentacene doped p-Terphenyl microcrystals — •Dominik Winter[1], Björn Ewald[1], and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The characteristic wavefunctions of the pentacene triplet states offer the possibility to maintain an asymmetric occupation of the various sublevels even at room temperature. Exposing pentacene single molecules embedded in a crystalline environment to microwaves of suited frequency, a controlled variation in population of the resonant triplet states can be achieved and optically detected - a technique termed optically detected magnetic resonance (ODMR). Here we report on our first results on the triplet polarization of pentacene doped p-terphenyl microcrystals prepared by microspacing in-air sublimation (MAS). By means of zero-field ODMR we analyze the microwave-induced transitions between the contributing triplet states. We will demonstrate and evaluate how the fast and easy method of MAS provides microcrystals that show an enhanced nuclear spin polarization. This process of triplet-induced dynamic nuclear polarization (DNP), is considered a potential approach to enhance the nuclear spin polarization of water and, thus, to significantly improve the image contrast of magnetic resonance imaging (MRI) as well as the sensitivity of non-invasive methods for structural characterization [1].

[1] K. Nishimura et al., Phys. Chem. Chem. Phys., 2019,21, 16408-16412

CPP 12.58 Mon 18:00 P1

Dye-induced Fluorescence Quenching of Quantum Dots having Different Excited State Lifetimes and Confinement Potentials — •Saleem Al-Maskari[1], Abey Issac[1], Eklas Al-Ghattami[1], SR Varanasi[1], R.G. Sumesh Sofin[1], and Osama K. Abou-Zied[2] — [1]Department of Physics, College of Science, Sultan Qaboos University, Muscat, 123, Oman — [2]Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, 123, Oman

We study the role of quantum confinement and the excited-state lifetime on the fluorescence quenching of heavy metal free quantum dots (QDs). Two different types of QDs are selected, namely CuInS2/ZnS (CIS) and InP/ZnS (InP). Quantum confinement in CIS QDs is weak (exciton Bohr radius aB = 4.3 nm versus particle size = 3.5 nm) whereas that in InP QDs is strong (aB = 15 nm versus particle size = 3.9 nm). Moreover, the excited-state lifetime of CIS QDs is ca. 298 ns whereas that of InP QDs is ca. 37 ns. Rhodamine 575 (Rh575) dye molecules adsorbed on the surface of QDs are used as the quencher. Stern-Volmer analysis of steady-state and time-resolved optical spectroscopy data reveal that in CIS-Rh575 and InP-Rh575 assemblies, although static and dynamic quenching are present, dynamic quenching is dominating. Further, quenching is more efficient in CIS-Rh575 assembly. We propose a model based on the quantum mechanical tunneling of the excited QD electron onto the dye induced surface states and subsequent non-radiative relaxation as the quenching mechanism. In addition, the long-lived excited state of CIS QDs support the tunneling mediated quenching in CIS-Rh575 assembly.

CPP 12.59 Mon 18:00 P1

sustainable materials for building-integrated photovoltaics —

•zimei chen[1], marie betker[1,2], constantin harder[1,3], benedikt sochor[1], matthias schwarzkopf[1], daniel söderberg[2], nadja kölpin[1], arik willner[1], and stephan v. roth[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), 22607 Hamburg, Germany — [2]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden — [3]Technische Universität München, 85748 Garching, Germany

Cellulose nanofibrils (CNF) as a bio-based material are very attractive due to their resource-saving and renewable property. They are biocompatible, flexible, lightweight, transparent and show excellent mechanical strength. With functionalized properties, they can be used as substrate for incorporating photovoltaic or electronic devices. In this project, we are going for building-integrated photovoltaics. Solar cells with PEDOT:PSS as electron blocking layer, P3HT:PCBM as photoactive layer and ZnO as hole blocking layer will be designed both in standard and inverted devices directly deposited on a CNF composite. A CNF / Ag nanowires mixture can be used as electrode material to improve the conductivity of Ag metal as electrode. Spray deposition will be used as a suitable technique to fabricate such functional layers in a large scale with homogeneous surface and a low roughness. in-situ grazing incidence small- and wide-angle X ray scattering (GISAXS/GIWAXS) will be used to observe the nanostructuring of each layer on the CNF composite base material and to optimize the fabrication process.

CPP 12.60 Mon 18:00 P1

P3HT:PCBM Polymer Solar Cells from a Didactive Perspective — •Shahidul Alam[1], Aman Anand[2], Md Moidul Islam[2], Rico Meitzner[2], Aurelien Sokeng Djoumessi[2], Josef Slowik[2], Zekarias Teklu[2], Peter Fischer[3], Christian Kästner[3], Jafar I. Khan[1], Ulrich S. Schubert[2], Frédéric Laquai[1], and Harald Hoppe[1] — [1]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Kingdom of Saudi Arabia — [2]Friedrich Schiller University Jena, Germany — [3]Ilmenau University of Technology, Germany

In this work, we studied the influence annealing process on the performance of the common polymer:fullerene bulk heterojunction solar cells with conventional architecture, comprising P3HT:PC60BM blend as a photoactive layer. The non-annealed active layer device exhibited a power conversion efficiency of less than 1%, which was significantly lower than the pre and post-annealed device. In order to investigate the impact of pre and post thermal annealing on the natural morphological state of the polymer, regiorandom and regioregular type P3HT were used in photoactive layers. Changes in solar cell performance were associated with different extraction probabilities due to changed annealing conditions. Several spectroscopic techniques like EL, SS-PL, and TR-PL were employed to comprehend the phenomenon of charge photogeneration processes. Finally, to explore the morphological changes upon annealing, AFM and ELI measurements were performed on films and solar cells, respectively.

CPP 12.61 Mon 18:00 P1

Simultaneously enhanced performance and stability of NFA solar cells with PETMP interfacial process — •Zerui Li[1,2], Changqi Ma[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]i-Lab &Printed Electronics Research Center, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences (CAS), Suzhou 215123, P. R. China

With the rapid development of novel non-fullerene acceptors (NFA), the PCE of NFA solar cells has reached over 18.6%, while the poor stability is still the limitation for application. For NFA solar cells, the hydroxyl radicals of ZnO forming under illumination would cause the degradation of the acceptor material, which is one key source for performance decrease. They could be effectively suppressed through modifying ZnO with radical trapping agents, such as 2-phenylethylmercaptan (PET). Unfortunately, PET is highly toxic with a bad smell. Here, PETMP with similar end group as PET is used as the alternative and it's found to be able to suppress the formation of hydroxyl radicals as well as to improve the device stability. Moreover, PETMP can improve the Jsc of devices through promoting the vertical phase separation of the active layer. Lastly, other similar derivatives is also tried and the amount of sulfhydryl is found to be highly important to the enhanced performance and stability, since only molecules with more sulfhydryl groups could work well. The interaction between PETMP and ZnO is the key factor promoting such a benefit. This work provides a perfect interfacial modification agent for more stable NFA solar cells.

CPP 12.62 Mon 18:00 P1

Improved hole extraction selectivity of polymer solar cells by combining PEDOT:PSS with WO3 — •Aurelien Sokeng Djoumessi[1,2], Shahidul Alam[1,2], Jose Prince Madalaimuthu[1,2], Aman Anand[1,2], Josef Slowik[1,2], Theo Pflug[3,4], Rico Meitzner[1,2], Roland Roesch[1,2], Enrico Gnecco[5], Alexander Horn[3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldstrasse 10, 07743 Jena, Germany — [3]Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Schillerstraße 10, 09648 Mittweida, Germany — [4]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Straße 70, 09126 Chemnitz, Germany — [5]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Löbdergraben 32, 07743 Jena, Germany

Since the device performance and stability of polymer solar cells strongly depend on the interfacial charge extraction layers, we investigated the impact of hole transport layer (HTL) in the devices by varying the HTL material and layer stack systematically between PEDOT:PSS and a sol-gel derived tungsten oxide (WO3). Interestingly there was an increase of the work function upon stacking both materials and the triple layer WO3/PEDOT:PSS/WO3 configuration resulted in the best device performance and an increased reproducibility in the lifetime compared to the use of pristine WO3 and PEDOT:PSS

CPP 12.63 Mon 18:00 P1

Compatible solution-processed interface materials for improving efficiency and prolonging the lifetime of polymer solar cells — •Zhuo Xu[1,2], Jose Prince Madalaimuthu[1,2], Josef Bernd Slowik[1,2], Rico Meitzner[1,2], Shahidul Alam[1,2,3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany. — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany. — [3]King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia

The electron transport layer in a solar cell is one of the main components which plays a crucial role in the separation of charges and improving the efficiency of the solar cells. Herein, solution-processed organic solar cells (PBDTTT-CT:PC70BM) were fabricated with PDINO, Titanium Oxide, and PDINO:TiOx as an ETL. The effect of different ETLs on the performance of solar cells was observed. An efficiency of 7.94% was achieved when PDINO:TiOx was used as an ETL which is one of the highest reported efficiencies for halogen-free solvent processed PBDTTT-CT:PC70BM polymer solar cells. Meanwhile, lower recombination and higher exciton dissociation probability were observed in PDINO:TiOx based PSCs, as well as the superior stability at 45 oC in air.

CPP 12.64 Mon 18:00 P1

Investigation of solvent dependent morphology degradation of PTQ-2F:BTP-4F bulk heterojunctions — •Lukas V. Spanier[1], Renjun Guo[1], Julian E. Heger[1], Yuqin Zou[1], Matthias Nuber[2], Matthias Schwartzkopf[3], Hristo Iglev[2], Reinhard Kienberger[2], Stephan V. Roth[3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Physik-Department, LS Laser- und Röntgenphysik, 85748 Garching — [3]DESY, 22607 Hamburg — [4]MLZ, TU München, 85748 Garching

Lately, organic solar cells (OSCs) have gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their manufacture. To make the manufacturing process of the bulk-heterojunction (BHJ) more environmentally friendly, increased efforts have recently been made to use halogen-free solvents, which, however, can lead to reduced efficiencies.

We investigate and compare the changes in morphology and performance stability of PTQ10:BTP-4F OSCs processed from various solvents, utilising operando grazing-incidence small and wide angle X-ray scattering during illumination and solar cell operation. We further show the impact of solvent composition on the charge carrier generation in the respective BHJs using time-resolved transient absorption spectroscopy, analysing the connection between thin-film morphology and device performance in polymer:non-fullerene acceptor OSCs.

CPP 12.65 Mon 18:00 P1

Polysulfobetaines as electron transport layers in organic solar cells employing a PBDBTCl-DTBT:BTP-4F active layer — •Sebastian Coen[1], Apostolos Vagias[2], Johanna Eichhorn[3], Lukas Spanier[1], Zerui Li[1], Xinyu Jiang[1], André Laschewsky[4,5], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching — [3]WSI, TU München, AG Experimentelle Halbleiterphysik, 85748 Garching — [4]Universität Potsdam, Institut für Chemie, 14476 Potsdam-Golm — [5]Fraunhofer IAP, 14476 Potsdam-Golm

Zwitterionic polymers (e.g. polysulfobetaines) have so far been systematically explored as antifouling agents due to their total electroneutrality and superhydrophilicity. These macromolecules carry a permanent dipole moment because of the simultaneous presence of positive and negative charges on the backbone. However, this dipole moment can affect the optoelectronic properties and charge transport when such polymers are considered as interlayers for organic solar cells. So far, the role of polyzwitterions as interlayers of organic photovoltaics remains unexplored. We investigate the use of one specific polysulfobetaine (PSPE) in this work. We study its optoelectronic and morphological properties under the aspect of usage in an organic solar cell. For this solar cell, we use an active layer of a PBDBTCl-DTBT:BTP-4F blend with an architecture of ITO/PEDOT:PSS/Active Layer/PSPE or PDIN/Ag. PDIN is a reference electron transport layer material showing similar band positions as PSPE.

CPP 12.66 Mon 18:00 P1

Possibilities and limitations for the alignment of polymer chains in photovoltaic materials — •Robin Teichgreber, Fabian Eller, and Eva M. Herzig — Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany

The arrangement of the polymer chains on the nanoscale in thin films influences the optical and electrical properties of the material in a decisive way. For efficient charge transport, a sufficient alignment of the polymers is necessary. Due to the sensitive nature of the microstructure to various influencing variables such as concentration, solubility, and temperature, this goal presents an experimental challenge. However, a deliberate alignment will allow to probe optical and electric photovoltaic properties more systematically. Li et al. [1] have shown that thin films with a high degree of alignment can be produced via dip-coating by varying the coating speed and concentration using the polymer PII-2T. The simple nature of the dip-coating process makes it attractive, also for other polymers, should similar results be obtainable. Here, it will be shown which results can be obtained in a dip-coating based process with P3HT and high performance polymers like PM6. For this purpose, different influencing variables such as coating speed, concentration, solvent quality and temperature are evaluated. In addition, the process is extended to include pre-processing and post-processing steps.

[1] Li, Qi-Yi; Yao, Ze-Fan; Lu, Yang; Zhang, Song; Ahmad, Zachary; Wang, Jie-Yu; et al. Adv. Electron. Mater., 6 (6), 2000080, 2020

CPP 12.67 Mon 18:00 P1

PbS quantum dot solar cells with a IZO buffer layer at quantum dot/ZnO interface — •Huaying Zhong[1], Wei Chen[1,2], Lukas V. Spanier[1], Christopher R. Everett[1], Manuel A. Reus[1], Xinyu Jiang[1], Shanshan Yin[1], Marlene Sophie Härtel[3], Jiahuan Zhang[3], Bertwin Bilgrim Otto Seibertz[4], Matthias Schwartzkopf[5], Stephan V. Roth[5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, 85748 Garching, Germany — [2]James-Franck-Straße 1 — [3]HZB, Solar Energy, 14109 Berlin — [4]TU Berlin, Department of Technology for Thin-film Components, 10623 Berlin — [5]DESY, 22607 Hamburg — [6]MLZ, TU München, 85748 Garching

Colloidal quantum dots (CQDs) have generated great interests in various optoelectronic devices due to their size-tunable bandgap, low-temperature solution processability. Lead sulfide (PbS) CQDs with large Bohr radius enable solar cells to harvest infrared photons of the solar spectrum beyond the absorption edge of crystalline silicon and perovskites. Interface engineering, as one of strategies to improve device performance, 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 sputter the indium zinc oxide (IZO) as the interlayer between PbS QDs absorption layer and ZnO nanoparticle (NP) electron transport layer (ETL), to fabricate PbS QD solar cells and study the trap densities and charge transport process at QDs interfaces.

CPP 12.68 Mon 18:00 P1

Preparation of Highly Crystalline ZnO Thin Films at Low Temperatures using ZnO Nanoparticles to Enable High-Quality Organic Solar Cells On Flexible Substrates — •Emanuel Anwander, Lukas V. Spanier, and Peter Müller-Buschbaum — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Franck-Straße 1, 85748 Garching

The possibility to build flexible light weight OSCs makes them very promising for aviation and aerospace applications. Therefore, inexpensive and scalable materials such as PET or PEN are desirable substrates. Conventional sol-gel preparation of ZnO thin films, which have proven to be the best choice for electron transport layers (ETLs) in inverted OSCs, requires annealing at temperatures up to 200°C. Since PET and PEN have glass transition temperatures of 69°C and 113°C, respectively, and are long term heat resistant at a maximum of 120°C and 155°C, respectively, a way to produce high-quality ZnO thin films at low temperatures is required. One approach to achieve this goal is to use a solution of pre-synthesized ZnO nanoparticles. These nanoparticles exhibit high crystallinity and thus good ZnO thin films that have higher charge carrier mobility and lower recombination rates than the sol-gel ZnO films can be formed at room temperature without annealing. This approach allows the realization of lightweight OSCs on flexible substrates that have the same or even higher efficiencies than conventional OSCs on rigid substrates with ETLs prepared using the sol-gel method.

CPP 12.69 Mon 18:00 P1

Calculation of vibronic progressions for PPE-PPV polymers — Montassar Chaabani[1], Samir Romdhane[1], and •Wichard Beenken[2] — [1]Laboratoire Matériaux Avancés et Phénomènes Quantiques, Faculté des Sciences de Tunis, Université Tunis El Manar, Campus Universitaire Tunis, 2092, Tunisia — [2]Institut für Physik, Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany

We have calculated the vibronic progressions for absorption and photoluminescence spectra of conjugated copolymers with alternating PPE and PPV units and various side-chains.

CPP 12.70 Mon 18:00 P1

Investigation of Crystal Structure 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 — [2]Applied Functional Polymers, University of Bayreuth

Polydiketopyrrolopyrrole (PDPP) copolymers are promising materials for applications in organic solar cells and transistors. Their chemical structure offers many possibilities for modifications, allowing to adjust their optoelectronic properties according to the desired application. Here, we investigated the molecular ordering and thermal properties in bulk (WAXS, DSC, TGA) and in thin films (GIWAXS, AFM) of three exemplary PDPPs, two donor polymers: PDPP$[T]_2\{2\text{-HD}\}_2$-T (PDPP$_T$) with thiophene flanking units and PDPP$[T]_2\{2\text{-HD}\}_2$-T{DEG} (PDPP$_{T-OEG}$) with thiophene flanking units and an additional OEG side chain, and one acceptor polymer: PDPP$[Py]_2\{2\text{-HD}\}_2$-T (PDPP$_{Py}$) with pyridine flanking units. In the ordered state, all three PDPPs show regular π-π-stacked backbones (d_{020} = 3.7 - 3.9 Å) and a regular layered structure of demixed backbones and side chains (d_{100} = 18.7 - 19.1 Å). While PDPP$_T$ and PDPP$_{T-OEG}$ only have sanidic liquid crystalline order, PDPP$_{Py}$ has a complex triclinic structure. PDPP$_{T-OEG}$ has the lowest melting temperature and PDPP$_{Py}$ the poorest thermal stability of the three. These results demonstrate the significant influence of seemingly small chemical modifications on crystal structure and thermal properties of PDPPs.

CPP 12.71 Mon 18:00 P1

Fluorinated thieno-quinoxalines - a systematic study on conformational locking and accompanied electronic characteristics — •M.M. Islam[1,2], A.M. Anton[1,2], R. Meitzner[1,2], C.L. Chochos[3,4], U.S. Schubert[1,2], and H. Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller

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Low band-gap thieno-quinoxaline derivatives are promising donor materials in organic solar cells. Fluorination, on the one hand, can lower both the HOMO as well as LUMO energy levels and thus enhance stability. On the other hand, electron exchange between hydrogen or sulfur and fluorine atoms might cause noncovalent interactions and steric hindrance. Six thieno-quinoxaline derivatives with systematically fluorinated sites have been investigated in solution, pristine films, and blends with ITIC as acceptor. UV-Vis absorption spectra reveal the sensitivity of stacking depending on the particular fashion of fluorination, which affects the size of photochromic units. The stacking propensity is corroborated by DFT simulations. Fluorescence spectroscopic indicates different photoluminescence pathways indicated by excitation-independent and excitation-selective PL signals.

CPP 12.72 Mon 18:00 P1

Optically detected magnetic resonance of OLED materials using a confocal microscope — •Pascal Schady, Fabian Binder, Mona Löther, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Optically detected magnetic resonance (ODMR) is a specialized technique to investigate spin-dependent optical transitions in solids. This method is also applicable for examining photoluminescence characteristics of semiconducting organic materials which are becoming increasingly popular for, e.g. display applications. In typical ODMR setups a laser beam is guided into a microwave-cavity from one side while the emission spectrum of the sample is detected from the other. To improve upon that, we build a confocal microscope around the cavity, such that white light as well as a laser beam are guided through the cavity opening onto the sample, allowing us to locally excite sample spots while monitoring the laser spot and photoluminescence through a camera and photodetector. By implementing these upgrades we aim to enhance sensitivity while also enabling improved control over the investigated sample spot in order to highlight excited state spin physics processes of potential organic light emitting diode materials.

CPP 12.73 Mon 18:00 P1

Conception and realization of a highly automated physical vapor deposition system for the fabrication of organic light-emitting diodes — •Fabian Binder, Mona Löther, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) are most commonly produced in ultra-high vacuum by physical vapor deposition of different organic and metallic layers on a carrier substrate. We designed a production system that should enable an almost completely automated production of the OLED-devices by the use of many sensor solutions and electric stepper motors. The different stepper motors allow a smooth and precise positioning of the OLED-sample above the evaporation crucibles in the vacuum chamber. Being positioned over an evaporation crucible, the sample needs to rotate with a defined speed to achieve an even deposition of the material. In order to vapor-deposit material, a certain, material-specific temperature range is required. This is realized by a software-based temperature controller which manages the evaporation rate according to the specifications of the user. A user interface makes it possible to design the desired OLED layer stack and provides information about the production progress. Finally, the first OLED devices will be produced and an electrical characterization of these devices, such as an investigation on the quantum efficiency will be done.

CPP 12.74 Mon 18:00 P1

Nanoscale alignment and chemical characterization of self-assembled all polymer donor-acceptor blends — •Dijo Moonnukandathil Joseph[1,2], Juanzi Shi[3], Wanzhu Cai[4], Hardik Gadher[1], Mohammad Soltaninzehad[1,2], Ivan G. Scheblykin[3], and Daniela Täuber[1,2] — [1]Leibniz Institute of Photonic Technology, Jena — [2]Friedrich-Schiller University Jena, Germany — [3]Lund University, Lund, Sweden — [4]Jinan University, Guangzhou, China

Control of light polarization properties in self-assembled all-polymer donor-acceptor blends enables intrinsic polarization-sensitive applications in organic optoelectronics. In general, the polarization properties of thin conjugated polymer films are related to the polymer chain alignment in the film. Macroscopic domains of polymer alignment were demonstrated in thin films of a quinoxaline-thiophene copolymer (TQ1), which had been self-assembled via floating film transfer [1]. The nano-chemical characterization of thin polymer films can be achieved by nano-infrared spectroscopy (NanIR) methods [2]. We use 2D polarization imaging for characterizing the polarization properties of several thin polymer blend films fabricated via floating film transfer. In addition we investigate the chemical nanostructure of these films using mid-infrared photoinduced force microscopy. – [1] Täuber et al. ACS Omega 2017, 2 , 32-40. [2] L. Xiao, Z.D. Schultz, Anal. Chem. 2018, 90 (1), 440-458.

CPP 12.75 Mon 18:00 P1

Ground-state charge transfer and influence on charge carrier transport in organic donor-acceptor mixtures — •Hongwon Kim[1], Florian Fenzel[1], Domenik Vögel[1], Andreas Opitz[2], and Wolfgang Brütting[1] — [1]Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg — [2]Supramolekulare Systeme, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

In organic semiconductors, charge transfer (CT) states form at interfaces or in mixtures of electron accepting and donating molecules. Their mutual electronic interaction is accompanied by a partial or full transfer of electric charges. This charge transfer is crucial to generate excess charges in (opto-)electronic devices, i.e. to facilitate electrical doping.

We have investigated donor-acceptor thin films consisting of electron donating molecules (DIP, 6T, DBTTF, and DBP) mixed with strong acceptors (F6TCNNQ and HATCN). It is investigated that the thermal activation energy (Ea) decreases and the electrical conductivity (σ) increases through doping by strong acceptors. Furthermore, the formation of CT states accelerates this doping effect and a highly improved conductivity can be obtained on DBTTF/F6TCNNQ as well as DIP/F6TCNNQ mixed thin films. This high conductivity is a result of increased concentration of charge carriers by doping effect as well as its improved mobility by CT states formation. However, the formation of CT states also has characteristic spectroscopic signatures and affects the growth behavior of molecular donor-acceptor blends.

CPP 12.76 Mon 18:00 P1

Morphology and stability study of organic thin films — •Meike Kuhn[1], Chris McNeill[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group,Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton

New, promising materials with high efficiency are constantly being discovered for organic solar cells. Often, these materials are chosen to mainly maximize efficiency. However, stability also plays an important role when selecting promising materials. The stability of organic materials depends on many variables, such as photochemical stability, photostability and morphological stability. In this analysis, we will attempt to gain a better understanding of nanostructural changes and hence morphological stability. [1] Using GIWAXS and absorption measurements, we systematically investigate how the ageing process affects the structure. In particular, we investigate the behaviour of the morphological ageing mechanisms, such as the orientation and aggregation of the material, as a function of temperature and substrate properties. These experiments are carried out on organic polymers such as PM6.

[1] C. Wöpke; C. Göhler; M. Saladina; X. Du; L. Nian; C. Greve; C. Zhu; K. M. Yallum; Y. J. Hofstetter; D. Becker-Koch; N. Li; T. Heumüller; I. Milekhin; D. R. T. Zahn; C. J. Brabec; N. Banerji; Y. Vaynzof; E. M. Herzig; R. C. I. MacKenzie; C. Deibel, Nat. Comm., accepted

CPP 12.77 Mon 18:00 P1

Photoluminescence and Quantum Yield of a deep blue TADF emitter — •Mona Löther, Fabian Binder, Pascal Schady, Jeannine Grüne, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light-emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) are becoming increasingly important due to their advantages over OLEDs of earlier generations as they enable access to triplet excitons via reverse intersystem crossing (rISC) without the need of resources-limited rare metal complexes. However, TADF OLEDs have yet to reach commercial viability, as an efficient and durable blue OLED remains to be found. A promising design for a blue host-dopant system is N7,N7,N13,N13,5,9,11,15-octaphenyl-5,9,11,15-tetrahydro-5, 9,11,15-tetraaza-19b, 20b diboradinaphtho[3,2,1-de:10, 20, 30-jk]pent-acene-7,13-diaminel (ν-DABNA). This system belongs to the multiresonant TADF compounds, represented typically by narrow band emission, high photoluminescence quantum yield (PLQY) and a small singlet-triplet gap ΔE_{ST}. In order to characterize its optical properties we examined the steady state photoluminescence (PL), transient photoluminescence (trPL) and PLQY. Furthermore, we used different host systems to survey the behavior of ν-DABNA in a host-emitter system. With these optical characterization methods we are able to better understand the promising candidate of TADF OLEDs with high efficiencies and color purity.

CPP 12.78 Mon 18:00 P1

Towards efficient blue perovskite lead-halide nanocrystal light emitting diodes — •Tassilo Naujoks[1], Adrian Hochgesang[2], Christopher Kirsch[3], Marcus Scheele[3], Mukundan Thelakkat[2], and Wolfgang Brütting[1] — [1]Institut für Physik, Universität Augsburg, Germany — [2]Universität Bayreuth, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany

The research focus for affordable solution-processed light-emitters has been shifted towards quantum-dot materials in recent years. High quantum yields (QY) even with inorganic nanocrystals (NC) capped by organic ligands have been achieved. One prominent, particularly highly luminescent type of NC is lead-halide perovskite with tunable colour by halide composition achieving near-unity QY.

While for red and green emitting NCs the quantum efficiency in the resulting LEDs is engineered to a satisfactory level, blue perovskite NCs are still underperforming. One issue with blue and therefore wider bandgap NCs lies in the very deep valence level. With that, hole injection into the NCs is significantly impaired. Here we present two approaches to enhance hole-injection into blue LHP NCs. The use of carbazole moieties either within the ligand on the NC surface or as a TCTA-doped polyvinyl-carbazole (PVK) polymeric hole transport layer increases the efficiency in perovskite NC LEDs. We propose that the carbazole group effectively blocks electrons, while its deep HOMO facilitates the injection into the similarly deep valence level of the blue perovskites.

CPP 12.79 Mon 18:00 P1

Photoinduced metastable and trapped charge-carrier pairs in neat amorphous films of OLED host materials — Sebastian Lulei[1], Jeannine Grüne[1], Andreas Sperlich[1], •Vladimir Dyakonov[1], Andrei Stankevych[2], Andrey Kadasshchuk[2], and Anna Köhler[2] — [1]Experimental Physics 6, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Soft Matter Optoelectronics and Bavarian Polymer Institute (BPS), 95448 Bayreuth

We discuss light-induced ESR (LESR) transients, PL-detected magnetic resonance (PLDMR), and thermally-stimulated luminescence (TSL) in neat amorphous thin films of 3’,5-di(9H-carbazol-9-yl)-[1,1’-biphenyl]-3-carbonitrile (mCBP-CN), which is commonly used as a host material for blue emitters based on thermally activated delayed fluorescence (TADF) in OLED devices. While the half-field LESR signal associated with triplet excitations shows fast saturation being comparable with the triplet lifetime, the full-field LESR featured extremely slow kinetics of both growth and decay at T=10K. The latter implies very slow accumulation and subsequent recombination of the photogenerated charge carriers due to shallow charge trapping at such low temperatures. These results are in good agreement with the observation of a long isothermal afterglow lasting up to thousands of seconds at 5K. Further, the persistent LESR signal is detected in the same temperature range as the TSL emission, implying that both are caused by the same trapped carriers. Finally, PLDMR showed signals from closed-by triplet states, emitting through fluorescence.

CPP 12.80 Mon 18:00 P1

Graphene nanoribbons synthesized on Au(111) and Au(788) in ultra-high vacuum conditions and by atmospheric pressure chemical vapor deposition method — •Vasilii Osipov, Yi Han, Philipp Weitkamp, Max Reimer, Dirk Hertel, and Klaus Meerholz — Chemistry department, University of Cologne, Germany

Graphene nanoribbons (GNRs) are an interesting class of materials due to their tunable width- and edge-type-dependent electronic structure. The state-of-the-art methods of GNRs synthesis are bottom-up processes involving polymerization of precursor molecules at catalytic surfaces, and are typically performed either in ultra-high vacuum (UHV) conditions or by atmospheric pressure chemical vapor deposition (AP-CVD) technique. Despite leading to GNR layers of reduced quality, the AP-CVD method possesses advantages of simplicity and better scalability compared to the UHV one, which make it a promising option for developing routes for synthesis of new types of GNRs. We present results of AP-CVD synthesis of GNRs from different precursors and their comparison to GNRs of corresponding types obtained by UHV method, using Raman spectroscopy. Particularly, degree of GNRs growth geometrical anisotropy, induced by using Au(788) growth substrate instead of Au(111), is investigated by observing the polarization-angle-dependent Raman intensity. This should eventually contribute to better understanding of the processes of GNRs synthesis and to development of technologies for functional (templating) materials for organic electronics.

CPP 13: Charged Soft Matter, Polyelectrolytes and Ionic Liquid

Time: Tuesday 9:30–11:15 Location: H38

Invited Talk CPP 13.1 Tue 9:30 H38

Insights into degradation mechanisms in Li-based batteries and advantages of polymer coatings — •Neelima Paul — Heinz Maier-Leibnitz Zentrum (MLZ), TU München, Lichtenbergstr. 1, 85748 Garching, Germany

Lithium-ion batteries are present in portable electronics, electric vehicles and grid-scale energy storage and are an inherent part of our daily life. They offer high energy density, high power density, stable temperature performance, and are safe. However, they eventually suffer from capacity fade due to some intrinsic degradation mechanisms, and thus have a limited cycle life. To increase their lifetime, knowledge of the responsible degradation/aging mechanism is crucial and most beneficial if determined without destructive disassembly of the battery. I will demonstrate how parameters responsible for aging such loss of mobile Li inventory, active material degradation, metallic Li plating, can be monitored and quantified using both operando and post-mortem neutron techniques. Thereafter, I will describe the main degradation mechanism in Li-metal batteries and show how this can be overcome by applying viscoelastic polymer coatings with a specific mechanical strength to the anode surface.

CPP 13.2 Tue 10:00 H38

Electrostatically Cross-Linked Reversible Gels - Effects of pH and Ionic Strength — Roman Staňo[1,4], •Peter Košovan[1], Andrea Tagliabue[2], and Christian Holm[3] — [1]Faculty of Science, Charles University, Prague, Czechia — [2]Universitá degli Studi dell Insubria, Como, Italy — [3]Institute for Computational Physics, University of Stuttgart, Germany — [4]University of Vienna, Austria

Mixing of oppositely charged macromolecules can lead to the formation of electrostatically cross-linked coacervate gels. In this simulation study, we determine the conditions under which four-armed star copolymers with charged end-blocks are able to form such coacervate gels. The cationic charged blocks consist of quenched charges, whereas the anionic blocks contain pH-responsive weak acid groups. We used the Grand-reaction method to determine the phase stability, equilibrium composition, and structural properties of these systems in equilibrium with a supernatant solution at various pH levels and salt concentrations. Depending on the pH and hence on the charge state of the polyanion blocks, we observed the emergence of three regimes: a solution, a sol of isolated star clusters, and a gel*percolating network of stars. Moreover, we demonstrate that the charge state of the stars in the gel phase can be well described by the ideal Henderson-Hasselbalch (HH) equation, despite the presence of strong interactions violating ideality. We can explain this surprising result by cancellation of two stongly non-ideal effects. This observation explains why various experiments on coacervate gels can be well described by the HH equation, although its assumption of ideality is violated.

CPP 13.3 Tue 10:15 H38

Temperature Dependence of PSS diffusion in multilayers of entangled PDADMA: more than one diffusion constant — •Annekatrin Sill[1], Peter Nestler[2], Peter Thran[1], and Christiane A. Helm[1] — [1]University of Greifswald, Institute of Physics, D-17489 Greifswald, Germany — [2]ZIK HIKE-Biomechanics, University of Greifswald, D-17489 Greifswald, Germany

Layer-by-layer assembly is a widely used tool for engineering materials and coatings, but the dynamics of the constituent polymer chains remain poorly understood. Using neutron reflectivity, the vertical diffusion of polyanion PSS (Mw(PSS) = 75.6 kDa) within PSS/PDADMA (Mw(PDADMA) = 72.1 kDa) multilayers is probed while annealing in 1 M NaCl solution at different temperatures. The observed diffusion could not be described by a simple diffusion model. Instead, two different PSS fractions (one mobile and one almost immobile, i.e. different diffusion constants) are the simplest model to describe the time dependence of the scattering length density profiles. Increasing the annealing temperatures (20 - 50 °C) increases the diffusion constant of both the fast and slow PSS fraction. Additionally, the fraction of fast PSS molecules is increased. We suggest that an immobile or nearly immobile fraction of polyelectrolytes is always present when the polymer length is beyond the entanglement limit and the sticky reptation model fails.

CPP 13.4 Tue 10:30 H38

Ratcheting charged polymers through symmetric nanopores using pulsed fields: Designing a low pass filter for concentrating DNA — •Le Qiao and Gary W. Slater — Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada

Size-based separation of DNA molecules is crucial for molecular analyses such as genome sequencing. To date, gel electrophoresis is the most commonly used separation method in the laboratory. However, due to poor resolution for larger molecules and difficult sample recovery, it cannot meet the goal of bulk separation. Alternatively, micro/nanofluidics offers a relatively inexpensive, label-free, and continuous separation with high throughput. In this talk, I will present a new proof-of-concept idea for the separation of DNA by contour length using a nanofluidic ratchet by combining nanopore translocation and pulsed fields. Using Langevin dynamics simulations, we show that it is possible to design pulsed fields to ratchet semiflexible molecules such that only short chains are successfully translocated, effectively turning the nanopore process into a molecular low-pass filter. The process itself can be performed with many pores in parallel, and it is possible to integrate it directly into nanopore sequencing devices, increasing its potential utility.

CPP 13.5 Tue 10:45 H38

Tuning water-in-salt electrolytes: impact of concentration and anion structure on local and long-ranged dynamics probed by NMR — •Dominik Gappa, Elisa Steinrücken, Manuel Becher, and Michael Vogel — TU Darmstadt, Institut für Physik kondensierter Materie, Darmstadt, Germany

Water-in-salt electrolytes (WiSE) are highly concentrated aqueous solutions of (Li-)salts. Newly developed WiSE, as they are non-flammable, nontoxic, have a high lithium-ion density and a wide electrochemical stability window (ESW), are promising materials for applications as lithium-ion electrolytes. Due the high amount of the solute and, thus, strong electrostatic interactions between the components they show complex molecular dynamics. A full understanding of interaction mechanism, e.g. the impact of the concentration and anion structure on the dynamics is still elusive. We investigate LiTFSI, which has a wide ESW for different salt concentrations in water. In particular, we exploit the isotope selectivity of Nuclear Magnetic Resonance (NMR) to observe the behavior of the constituents of LiTFSI-H_2O mixtures with various concentrations separately via ^{1}H, ^{7}Li and ^{19}F NMR. The anion structure is modified by extending one side group of the originally symmetric TFSI anion, leading to increasingly heterogeneous dynamics. Local dynamics are investigated by spin-lattice relaxation, including field-cycling NMR, and long-ranged transport by diffusion experiments. Rotational correlation times and diffusion coefficients are extracted to scruntinize the validity of the Stokes-Einstein relation.

CPP 13.6 Tue 11:00 H38

Tuning the Electronic and Ionic Thermoelectric Transport Properties in Polymer Electrolytes by Carbon Based Additives — •Maximilian Frank[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Ionic transport constitutes a key process in organic-based electrochemical energy storage media. As such, it also offers intriguing possibilities for the utilization of these materials in thermoelectrics (TE) to recuperate waste heat into electrical power. In this work we present our results on the electrical and thermoelectrical characterization of a methacrylate based solution processable solid polymer electrolyte. By means of impedance spectroscopy over a broad frequency regime from 100 mHz up to 500 kHz and in a technologically relevant temperature range between 263 K and 363 K we investigate the dynamics of charge carriers in the solidified electrolyte. Furthermore, we demonstrate that the electronic and ionic transport properties can be efficiently varied by the ratio between Lithium-salt and carbon-based additives, in this case, carbon nanotubes. Even more, we can reverse the sign of the occurring thermovoltage, which allows for different TE operational modes depending on ambient temperature. A proof-of-concept all organic TEG verifies the functionality of our approach and, thereby, substantiates the potential of mixed ionic and electronic materials for future TE applications.

CPP 14: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Tuesday 9:30–11:15 Location: H39

CPP 14.1 Tue 9:30 H39

Where is the Water? — •Maximilian Fuchs[1,2], Eduardo Machado Charry[1,2], Gregor Böhm[1,2], Roland Resel[1], and Karin Zojer[1,2] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper, Graz University of Technology, Austria

The take up of liquid water by paper is a complex interplay between capillary transport and swelling of cellulose-lignin-based fibers. Though paper is a convenience product used every day, little is known how swelling affects the pore space between fibers and the subsequent transport within it. We used X-ray microcomputed tomography to monitor the spread of water in-situ. The sequence of 3D-images, segmented by a neural network, traces the time-dependent progression of swelling and liquid transport up to one hour after the application of water. We find that water not only swells the fiber walls, but also expands the pore space between the fibers. Even more remarkable is that there is no liquid water in the pores between the fibers of the examined paper. Rather, liquid water was found exclusively in the fiber lumen.

CPP 14.2 Tue 9:45 H39

Rational Design of Novel Photoswitches with Generative Models — •Robert Strothmann, Christian Kunkel, Johannes T. Margraf, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The sheer vastness of chemical spaces poses a daunting challenge to molecular discovery through high-throughput screening based on exhaustive sampling. Generative models (GMs) are an emerging machine learning (ML) approach that enables a more guided discovery. Implicitly learning chemical design rules from large reference data sets and suitable descriptors of a targeted functionality, GMs directly propose promising, yet diverse candidates.

Here we explore the use of GMs for the design of novel molecular photoswitches. In order to guarantee the desired functionality in the generated molecules, we specifically employ scaffold decoration methods that append chemically meaningful side-groups to a predefined photochromic core. In a second step, the creation process needs to be conditioned towards performant switching capabilities. In the absence of sufficient corresponding experimental reference data, this conditioning is based on synthetic first-principles data. To this end, we discuss computationally efficient descriptors assessing addressability and robustness.

CPP 14.3 Tue 10:00 H39

Transferable hidden variables in sequence space learned by transencoder neural networks — •Marco Werner — Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany

The relation between chemical sequences and the properties of polymers is investigated using artificial neural networks with a bottleneck layer of neurons. By training such AutoEncoder networks to translate between sequence and property (TransEncoder[1]), one may identify variables that control the physical relationship behind. Here, networks were trained to predict the effective free energy landscape of a copolymer interacting with a lipid membrane depending on its sequence of hydrophilic and hydrophobic monomers. TransEncoders that were split into separate encoder-decoder channels have learned to decompose the free energy into independent components that were physically meaningful. For instance, they reflect theoretical concepts such as solutions of the Edwards equation. Sequence-complete data sets for training were obtained via Rosenbluth sampling of single chains in a given density field. It is demonstrated that once the sequence patterns were learned based on the large data set for chain length $N = 14$, a small number of ~ 20 examples was sufficient to transfer-learn the prediction to a more detailed simulation model with explicit lipids and solvent (accuracy $0.5 k_B T$). The results open a perspective to physics-informed inverse searches, for instance, for copolymer sequences leading to the smallest translocation time through a membrane. [1] M. Werner, ACS Macro Lett. 10, 1333 (2021).

CPP 14.4 Tue 10:15 H39

Improved virtual orbitals for the calculation of X-ray absorption spectra for organic molecules — •Rolf Würdemann[1] and Michael Walter[2,3] — [1]Freiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — [3]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

X-ray absorption spectroscopy (XAS) is an element specific local probe used for the analysis of materials. One way to compare and interpret experimentally measured spectra is to perform ab initio calculations of XAS spectra for molecules in given geometries. This opens a way to distinguish between different isomers and gain a deeper understanding of the bonding situation.

Common ways to calculate XAS spectra by density functional theory (DFT) either utilize fractional charges in the frozen cores or restrict the state-space of linear time-dependent DFT. In our contribution we examine the possibility to utilize the combination of range-separated functionals (RSF) with Huzingas improved virtual orbitals to calculate XAS spectra. This combination has been successful in the calculation of charge transfer excitations[1].

[1] R. Würdemann, M. Walter, J. Chem. Theory Comput. 2018, 14, 7, 366

CPP 14.5 Tue 10:30 H39

Transport of organic volatiles through paper: physics-informed neural networks for solving inverse and forward problems — •Alexandra Serebrennikova[1,4], Raimund Teubler[2,4], Lisa Hoffellner[2,4], Erich Leitner[2,4], Ulrich Hirn[3,4], and Karin Zojer[1,4] — [1]Institute of Solid State Physics, TU Graz, Petersgasse 16, Graz, 8010, Austria — [2]Institute of Analytical Chemistry and Food Chemistry, TU Graz, Stremayrgasse 9/II, Graz, 8010, Austria — [3]Institute of Bioproducts and Paper Technology, TU Graz, Inffeldgasse 23, Graz, 8010, Austria — [4]Christian Doppler Laboratory for mass transport through paper, Petersgasse 16, Graz, 8010, Austria

Transport of volatile organic compounds (VOCs) through porous media with active surfaces takes place in many applications, e.g., in cellulose-based materials for packaging. To date, mathematical models proposed in literature for this complex process are scarce and have not been systematically compiled together with experimental data.

Based on a model for water-vapor transport through paper (Ramarao et al. (2003)), we propose to describe transport of VOCs via diffusion in pores and sorption to fibers. It is key to determine the necessary material parameters for the model. Using experiments for that is challenging, as the related system of non-linear PDEs does not offer analytical solutions.

We demonstrate for dimethyl sulfoxide and n-tetradecane, how combining experimental concentration data with physics-informed neural networks yields these parameters as solution of an inverse problem.

CPP 14.6 Tue 10:45 H39

STED-Inspired Sub Diffractional Cationic Lithography — •Sourav Islam[1], Marco Sangermano[2], and Thomas Klar[1] — [1]Institute of Applied Physics, Johannes Kepler University Linz, 4040 Linz, Austria — [2]Department of Applied Science and Technology, Politecnico Di Torino, Torino, Italy

Cationic polymerization has come out as a low cost, efficient, biocompatible alternative to radical polymerization because of lower toxicity of the monomers, lower shrinkage stress, no oxygen inhibition. Although the mechanism of cationic polymerization is well understood(1), the knowledge about two-photon induced cationic polymerization is still insufficient. In our work, we try to fill the void in the knowledge of two photon induced cationic polymerization and the scope of STED-inspired (2) sub diffractional lithography. 3,4-Epoxycyclohexylmethyl 3,4 epoxycyclohexanecarboxylate (CE) was used as monomer and Triarylsulfonium hexafluoroantimonate salts and 2-Isopropylthioxanthone (ITX) were used as onium salt and photosensitizer, respectively. 110fs laser pulses of 780nm wavelength were used to write two-photon polymer lines with a feature size of 315nm. Furthermore, 60% suppression of polymerization was achieved using an additional 660nm continuous beam overlapped with 780nm beam. To obtain further reduction of the feature size, a donut shaped beam profile was produced by installing a 2-pi phase plate in the 660 nm beam path. This way, lines of 195 nm feature size were achieved. 1.M. Sangermano Pure and Applied Chemistry, 84, 2089 (2012). 2.Fischer, Wegener, Opt. Mat. Exp. 1, 614 (2022)

CPP 14.7 Tue 11:00 H39

Photoluminescence spectroscopy for the detection of microplastics - the Nile Red approach — •Srumika Konde, Stefan Brackmann, Marina Gerhard, and Martin Koch — Department of Physics and Material Sciences Center, Philipps-University of Marburg, Germany

For the detection and classification of microplastics, most researchers commonly use FTIR or Raman spectroscopy. These state-of-the-art methods are, however, laborious, cost-intensive, and time-consuming. To establish a less arduous and inexpensive approach, we propose photoluminescence-based multispectral imaging. Based on the parallel research in our workgroup, we have found that the autofluorescence of plastics lies predominantly in the UV region. To accommodate the identification in the visible region we use a solvatochromic dye called Nile Red. PLE/PL spectra of stained plastics and stained natural materials have been analyzed to determine the right excitation and emission windows for building an imaging system. This analysis has been performed using LDA (linear discriminant analysis). Based on our analysis we propose a system consisting of a blue excitation LED, an RGB camera, and two bandpass filters which would yield about 98% accuracy in isolating plastics from natural materials.

CPP 15: 2D Materials 4 (joint session HL/CPP/DS)

Time: Tuesday 9:30–12:00 Location: H36

Invited Talk CPP 15.1 Tue 9:30 H36

Ultrafast all-optical modulation and frequency conversion in 2D materials — •Sebastian Klimmer[1], Artem Sinelnik[1,2], Isabelle Staude[1,2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Germany

Large efforts have been devoted in the last years to realizing nonlinear integrated devices for frequency conversion, sensing, signal modulation and quantum optics. Two-dimensional (2D) materials, such as graphene and transition metal dichalcogenides (TMDs), provide distinct advantages in this respect thanks to their ease of integration on photonic platforms[1] and their atomically thin nature, which relaxes phase matching constraints and thus offers a practically unlimited bandwidth for nonlinear optical effects [2]. In this seminar I will present our recent results in the field of nonlinear optics with 2D materials, including ultra-broadband four-wave mixing in the telecom range, ultrafast all-optical modulation of second- and third-harmonic generation in TMDs[3] and graphene and ultrafast polarization-resolved second-harmonic spectroscopy to probe the valley degree of freedom in TMDs.

[1] He, J. *et al.*, Nano Lett. **21**, 7, 2709-2718 (2021)
[2] Trovatello, C. *et al.*, Nat. Photonics. **15**, 6-10 (2021)
[3] Klimmer, S. *et al.*, Nat. Photonics. **15**, 837-842 (2021)

CPP 15.2 Tue 10:00 H36

strain tuning of exciton and trion dynamics in monolayer WSe2 at cryogenic temperatures — •zhao an[1], pedro soubelet[2], andreas v. stier[2], michael zopf[1], yaroslav zhumagullov[3], jaroslav fabian[3], paulo e. faria jonior[3], jonathan j. finley[2], and fei ding[1,4] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, 85748 Garching, Germany — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [4]Laboratorium fur Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Transition metal dichalcogenides (TMD) receive increasing attention these years. In TMD monolayers, the light-matter interaction is driven by strong excitonic effects. Additional to neutral excitons, singlet/ triplet trions are observed, in which the additional charge is either in the same or opposite valley with respect to excitons. We apply dynamic strain at cryogenic temperatures to investigate the exciton dynamics of monolayer WSe2. Biaxial strain is electrically controlled via a piezoelectric actuator and transferred to the hBN/WSe2/hBN. We find that next to changes in the emission energy and intensity, the singlet-triplet trion fine structure is affected. Polarization-resolved PL spectroscopy reveals that biaxial strain alters the polarizations of trions, which is attributed to changes in the pumping of resident electrons and the intervalley scattering of excitons and electrons.

CPP 15.3 Tue 10:15 H36

Optical nonlinearities in the excited carrier density of 2d TMDs — •Daniel Erben[1], Alexander Steinhoff[1], Michael Lorke[1,2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen — [2]Bremen Center for Computational Materials Science, University of Bremen

The prospects of using 2d transition metal dichalcogenides (TMDs) in future optoelectronic device application requires insight in the excitation dynamics of photoexcited charge carriers and the resulting optical nonlinearities. Utilizing ab-initio electronic-state calculations combined with many-body treatment of optical excitation, we calculate the excited carrier dynamics and the nonlinear absorption in MoS_2, $MoSe_2$, WS_2, and WSe_2 under various excitation conditions.

We find, that the increase of the carrier density with excitation strength deviates from a linear behaviour. Based on this, the validity range of a linear approximation for the excited carrier density as function of the pump fluence is determined. The use of a linear absorption coefficient of the unexcited system can significantly underestimate the achievable carrier density for strong pump fields. Furthermore, we study the excitation-induced many-body effects of excited charge carriers like band-gap renormalization, dephasing, screening, and scattering processes, that are mediated by the strong Coulomb interaction. Additional contributions to optical nonlinearities originate from phase space filling.

15 min. break

CPP 15.4 Tue 10:45 H36

Second order coherence of a condensate of exciton-polaritons in an atomically thin crystal — •Jens-Christian Drawer[1], Hangyong Shan[1], Sven Höfling[2], Carlos Anton-Solanas[3], Martin Esmann[1], and Christian Schneider[1] — [1]Universität Oldenburg, Germany — [2]Universität Würzburg, Germany — [3]Universidad Autónoma de Madrid, Spain

We study the second order coherence of a condensate of exciton-polaritons emerging in a microcavity loaded with an atomically thin $MoSe_2$ crystal. Under cryogenic temperatures, angle-resolved PL and reflectivity measurements reveal the formation of two polariton resonances, as the hallmark of the strong coupling regime. The characteristic condensation threshold manifests via the nonlinear input-output-characteristics of the emission. In order to gain deeper information about the photon statistics emitted from the cavity, we perform the Hanbury Brown- and Twiss experiment as a function of the polariton occupation in the effective ground state. While the emission features a bunching effect below threshold, hinting at a thermal contribution of the polariton emission, above threshold the second order correlation transits towards $g^{(2)}(\tau = 0) = 1$, which is indicative for the formation of a coherent state in the quantum optical sense.

CPP 15.5 Tue 11:00 H36

Theoretical description of moiré excitons in twisted $MoSe_2$ homobilayers — •Ruven Hübner[1], Malte Kremser[2], Viviana Villafañe[2], Marko M. Petrić[3], Matthias Florian[4], Alexander Steinhoff[1], Mackillo Kira[4], Nathan P. Wilson[2], Andreas V. Stier[2], Kai Muller[3], and Jonathan J. Finley[2] — [1]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [2]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [3]Walter Schottky Institut and Department of Electrical and Computer Engineering, Technische Universität München, Garching, Germany — [4]University of Michigan, Dept. of Electrical Engineering and Computer Science, Ann Arbor, MI, USA

By introducing a twist between multiple monolayers of transition metal dichalcogenides we can observe superstructures with a new periodicity - namely the moiré lattice. Its size depends on the twist angle and therefore offers the possibility to modify properties like exciton energies as a function of the twist angle. We demonstrate, how DFT calculations of an untwisted $MoSe_2$ bilayer allow us to locally model the band variation inside the moiré unit cell at all dominant high symmetry points of the Brillouin zone. The resulting model provides access to arbitrary moiré potentials experienced by different exciton species and allows us to calculate their twist angle dependent spectra. For all twist angles we assign the lowest energy to interlayer excitons formed between the Γ- and K-valley. The twist angle dependent shift of 5 meV per degree for small angles is in good agreement with experiment.

CPP 15.6 Tue 11:15 H36

Dielectric screening effects on the exciton binding-energy and exciton diffusion in a 2D material — •Lukas Gümbel, Philip Klement, and Sangam Chatterjee — Institute of Experimental Physics I and Center for Materials Research (ZfM/LaMa), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, Giessen D-35392, Germany

Two-dimensional semiconductors have proven to be candidates for numerous applications in the field of optoelectronics. Especially transition-metal dichalcogenides such as WS_2 have attracted extensive research due to the direct band-gap emerging in the monolayer limit. The optoelectronic properties are dominated by tightly-bound excitons denoted as A, B, and C. As the electric field lines of the excitonic states extend into the surrounding material, the energy states are subject to dielectric screening effects. Here we show that stronger dielectric screening equally shifts the excitonic ground state energies of the A-, B-, and C-excitons in WS_2 to lower energies. We find a shift of 20 meV in monolayers encapsulated in hBN and observe a non-hydrogenic Rydberg-series yielding a quasiparticle band-gap energy of 2.33 eV with an 1s excitonic binding energy of 0.30 eV. Additionally, we study exciton diffusion in different dielectric environments yielding a diffusion coefficient of 9 cm^2/s. These results complement the underlying theory and may pave the way to a deeper understanding of screening effects in various 2D-Materials.

CPP 15.7 Tue 11:30 H36

Brightening of a dark monolayer semiconductor via strong light-matter coupling in a cavity — •Hangyong Shan[1], Ivan Iorsh[2], Bo Han[1], Falk Eilenberger[4], Martin Esmann[1], Sebastian Klembt[3], Sven Höfling[3], Carlos Antón-Solanas[1], Ivan A. Shelykh[2], and Christian Schneider[1] — [1]Oldenburg University, Oldenburg, Germany. — [2]St. Petersburg, Russia — [3]Universität Würzburg, Würzburg, Germany — [4]Friedrich Schiller University, Jena, Germany

We study the modification of the material properties via strong coupling and demonstrate an effective inversion of the excitonic band-ordering in a monolayer of WSe2 with spin-forbidden, optically dark ground state. In our experiments, we harness the strong light-matter coupling between cavity photon and the high energy, spin-allowed bright exciton, and thus creating two bright polaritonic modes in the optical bandgap with the lower polariton mode pushed below the WSe2 dark state. We demonstrate that in this regime the commonly observed luminescence quenching stemming from the fast relaxation to the dark ground state is prevented, which results in the brightening of this intrinsically dark material. We probe this effective brightening by temperature-dependent photoluminescence, and we find an excellent agreement with a theoretical model accounting for the inversion of the band ordering and phonon-assisted polariton relaxation.

CPP 15.8 Tue 11:45 H36

Broadband pump-probe microscopy at 1.5 MHz repetition rate — •Devapriyo Mithun[1], Michael Frosz[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Max Planck Institute for the Science of Light, Erlangen, Germany

Ultrafast pump-probe spectroscopy is one of the most commonly used techniques to resolve photoinduced excited states dynamics: a pump pulse excites the system under investigation, which is then monitored by measuring the changes in the differential reflection (ΔR/R) of a temporally delayed probe pulse. Here, we discuss the realization of a pump-probe setup, which exhibits high sensitivity operating with a temporal resolution of $\approx$ 100 fs and spatial resolution of $\approx$ 3 μm with 515 nm pump and a broadband probe spectrum in the range 650-1000 nm, generated with a photonic crystal fiber.

We modulate the pump pulse at 1.5 MHz using an acousto-optic modulator. By doing this, we achieve a sensitivity, defined as the minimum detectable ΔR/R, of 10^{-7} at 10 ms integration time. Finally, we implemented a Fourier transform based interferometric detection scheme to achieve a fast measurement of ΔR/R over the entire broadband spectrum.

Our pump-probe setup provides a powerful tool for broadband pump-probe microscopy with high sensitivity and high temporal resolution, which is ideal for the study of nanostructures such as carbon nanotubes and layered materials.

CPP 16: Active Matter 2 (joint session DY/BP/CPP)

Time: Tuesday 10:00–13:00 Location: H18

CPP 16.1 Tue 10:00 H18

Density fluctuations in bacterial binary mixtures — •Silvia Espada Burriel, Victor Sourjik, and Remy Colin — Max Planck Institute for Terrestrial Microbiology, Karl-von-Frisch-strasse 10, 35043 Marburg & Center for Synthetic Microbiology (SYNMIKRO), Karl-von-Frisch-strasse 14, 35043 Marburg

In wild environments, bacteria are found as mixtures of motile and sessile species, which interact physically and chemically to give rise to complex community organization. Very little is understood of the role of physical interactions in these processes: Numerical works on dry active matter and experiments on colloidal systems have shown that the activity of the active particles may affect the spatial distribution of passive particles with which they are mixed. However, the physical behavior of binary mixtures of bacteria remains largely unexplored. In our study, we present a novel phenomenon in which non-motile bacteria form large density fluctuations when mixed with motile bacteria, distinct from the aforementioned behaviors. We systematically explored the phase diagram of the mixtures in experiments combining microfluidics, fluorescence (confocal) microscopy, quantitative image analysis and parameter tuning by genetic engineering. Our experimental results show that the emergence of these large density fluctuations of the non-motile cells in presence of motile cells is controlled by hydrodynamic interactions between the motile and non-motile cells and by the sedimentation of the non-motile cells, possibly because it breaks the systems symmetry.

CPP 16.2 Tue 10:15 H18

Pulsating Active Matter — •Yiwei Zhang and Etienne Fodor — 0 Av. de la Faiencerie, 1511 Luxembourg

Active matter features the injection of energy at individual level keeping the system out of equilibrium, which leads to novel phenomenologies without any equilibrium equivalents. So far, most active matter models assign a velocity to each particle, whilst we herein consider a system of pulsating soft particles where the activity sustains particles' periodic deformation instead of spatial displacement. At sufficiently high density, we reveal the existence of wave propagation independent of any particle migration, and derive the corresponding phase diagram. We study the character of phase transitions, and investigate the underlying physical mechanisms, using both particle-based simulations and hydrodynamic analysis.

CPP 16.3 Tue 10:30 H18

Long-Range Nematic Order in Two-Dimensional Active Matter — •Benoît Mahault[1] and Hugues Chaté[2,3] — [1]MPIDS, 37077 Göttingen, Germany — [2]SPEC, CEA-Saclay, 91191 Gif-sur-Yvette, France — [3]CSRC, Beijing 100193, China

Studies of active matter continue to flourish, exploring more and more complex situations in an increasingly quantitative manner. Evidence has accumulated that shows active matter exhibits properties that are impossible in thermal equilibrium or even in driven systems. In spite of all this progress, important fundamental questions remain open. Such a long-standing issue is whether true long-range nematic order can emerge in two space dimensions. In this talk, we will present theoretical and numerical results obtained from minimal models of self-propelled polar particles aligning nematically. Our study shows that the orientational order emerging from such systems is quasi-long-ranged beyond the scale associated to induced velocity reversals, which is typically extremely large and often cannot even be measured. On scales where particle motion is ballistic, nematic order appears truly long-range. A hydrodynamic theory for this de facto phase is derived, and we show that its structure and symmetries differ from conventional descriptions of both polar flocks and active nematics. Our analysis of this field theory predicts π-symmetric propagative sound modes and the scaling form of space-time fluctuations. Finally, numerical results confirm the theory and allow us to estimate all scaling exponents.

CPP 16.4 Tue 10:45 H18

Collective behavior of repulsive chiral active particles with non-reciprocal couplings — •Kim L. Kreienkamp and Sabine H. L. Klapp — Technische Universität Berlin, Germany

Mixtures of chiral active particles [1] as well as non-reciprocal systems [2] show intriguing collective behavior like pattern formation and traveling waves. The combination of both – non-reciprocal couplings in mixtures of chiral active particles – promises a rich variety of collective dynamics.

Here, we investigate how non-reciprocal couplings and naturally occurring repulsive interactions due to finite particle sizes affect the collective behavior in a mixture of two species of particles. We analyze the effects due to non-reciprocity and finite size individually as well as their interplay based on a field description of the system in terms of the particle concentration and director field, measuring the overall orientation of particles at a certain position.

We derive the field equations under the mean-field assumption by coarse-graining microscopic Langevin equations for individual chiral particles, which are modeled as self-propelling circle swimmers with soft repulsive forces, comprising the finite size effects. Particles of the two species rotate with different intrinsic frequencies and align with near-by particles. Focusing on non-reciprocity, we use a non-mutual alignment between the particles.

[1] D. Levis and B. Liebchen, Phys. Rev. E 100, 012406 (2019)

[2] M. Fruchart, R. Hanai, P. B. Littlewood, and V. Vitelli, Nature 592, 363-369 (2021)

CPP 16.5 Tue 11:00 H18

Memory-induced chirality in self-freezing active droplets — •Aritra K. Mukhopadhyay[1], Kai Feng[2], José Carlos Ureña Marcos[1], Ran Niu[2], Qiang Zhao[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, 64289 Darmstadt, Germany. — [2]Huazhong University of Science and Technology, 430074 Wuhan, China.

We experimentally realize and numerically model a new type of self-propelled droplet swimmer which exhibits chiral motion due to self-induced memory effects without requiring any explicit symmetry breaking caused by specific droplet geometries or complex environments. The droplets are composed of a binary polymer mixture that solidifies over time, simultaneously emitting certain polymers into their environment. A spontaneous asymmetry of the emitted polymer concentration along the stationary droplet surface induces Marangoni flows which cause the droplet to initially self-propel ballistically. However, the emitted polymers diffuse slowly and form long-lived trails with which the droplet can self-interact in the course of time and this leads to a dynamical transition from ballistic to chiral motion. The droplets persistently exhibit chiral motion with the same handedness until at even later times a second transition occurs when the droplets confine themselves leading to self-trapping over the timescale of our experiments and simulations. Our results exemplify a new route to realizing synthetic active particles whose dynamics can be controlled via the pronounced self-induced memory effects.

15 min. break

CPP 16.6 Tue 11:30 H18

Role of advective inertia in active nematic turbulence — •Colin-Marius Koch and Michael Wilczek — Theoretical Physics I, University of Bayreuth, Bayreuth

Suspensions of active agents with nematic interactions can exhibit complex dynamics such as mesoscale turbulence. Continuum descriptions for such systems are inspired by the hydrodynamic theory of liquid crystals and feature an advective nonlinearity which represents inertial effects. The typically low Reynolds number of such active flows raises the question whether and under which conditions the active stresses present in these systems can excite inertial flows. To address this question, we investigate mesoscale turbulence in a two-dimensional model for active nematic liquid crystals. In particular, we compare numerical simulations with and without nonlinear advection and frictional damping of the flow field. Studying the nondimensionalized equations of motion, we find that inertia can trigger large-scale motion even for small microscopic Reynolds numbers if the active forcing is sufficiently large and the Ericksen number is sufficiently low. Performing a spectral analysis of the energy budget, we identify an inverse energy transfer caused by inertial advection, whose impact is small in comparison to active forcing and viscous dissipation but accumulates over time. We additionally show that surface friction, mimicked by a linear friction term, dissipates the transported energy and suppresses the large-scale motion. We conclude that, without an a priori knowledge of model parameters matching experiments, including inertia and friction may be necessary for consistent modeling of active nematic turbulence.

CPP 16.7 Tue 11:45 H18

Pumping in active microchannels — •Goncalo Antunes[1,2,3], Paolo Malgaretti[1,2,3], Siegfried Dietrich[2,3], and Jens Harting[1,4] — [1]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IEK–11), Forschungszentrum Jülich, Erlangen, Germany — [2]Max–Planck–Institut für Intelligente Systeme, Stuttgart, Germany — [3]Universität Stuttgart, Stuttgart, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany

Much attention is currently being given to the problem of manipulating fluids at the microscale, with successful applications to fields such as 3D fabrication and biomedical research. Often micropumps are a fundamental component of these microfluidic systems. An intriguing technique to manipulate fluid flows in a channel is diffusioosmosis. Fluid flow is obtained upon imposing an inhomogeneous concentration of some solute, which generates flow in a boundary layer around the channel walls. This inhomogeneity is the result of a spatially inhomogenous production rate of solute inside the channel.

We show that a solute-producing, corrugated, active channel can act as a micropump even when it is fore-aft symmetric. This result is obtained by coupling the Stokes equation with an advection-diffusion equation for the solute concentration, which we solve analytically in the limit of thin, weakly-corrugated channels. Lattice Boltzmann simulations further support the existence of the symmetry-breaking. Our calculations are also valid for left-right asymmetric channels, and provide a tool to optimize the pumping rate of an active microchannel by tuning its shape or its solute production rate.

CPP 16.8 Tue 12:00 H18

Active Refrigerators Powered by Inertia — •Lukas Hecht[1], Suvendu Mandal[1], Hartmut Löwen[2], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Hochschulstr. 8, D-64289 Darmstadt, Germany — [2]Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

We present the operational principle for a refrigerator which uses inertial effects in active Brownian particles (ABPs) to locally reduce the (kinetic) temperature by two orders of magnitude below the environmental temperature. This principle requires two ingredients: First, we need the feature of inertial ABPs to undergo motility-induced phase separation into coexisting phases with different (kinetic) temperatures and second, a mechanism which localizes the dense phase in the targeted cooling domain is required.

Here, we exploit the peculiar but so-far unknown shape of the phase diagram of inertial ABPs to initiate motility-induced phase separation in the targeted cooling domain only. Remarkably, active refrigerators operate without requiring isolating walls separating the cooling domain from its environment. This feature opens the route towards using active refrigerators to systematically absorb and trap substances such as toxins or viruses from the environment.

CPP 16.9 Tue 12:15 H18

The influence of motility on bacterial accumulation in a microporous channel — •Christoph Lohrmann[1], Miru Lee[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37073 Göttingen, Germany

Swimming microorganisms are often encountered in confined geometries where also an external flow is present, e.g. in filters or inside the human body. To investigate the interplay between microswimmer motility and external flows, we developed a model for swimming bacteria based on point coupling to an underlying lattice Boltzmann fluid. Random reorientation events reproduce the statistics of the run-and-tumble motion of the bacterium E. coli. We present the application of the model to the study of bacterial dynamics in a channel with a single cylindrical obstacle. In accordance with experimental measurements, simulations show asymmetric accumulation behind the obstacle only when the bacteria are active and an external flow is present.

Lee, Miru *et al.*, *Soft Matter* **17**, 893-902 (2021)

CPP 16.10 Tue 12:30 H18

Inertial dynamics of an active Brownian particle* — •Jonas Mayer Martins and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Active Brownian motion commonly assumes spherical overdamped particles. However, self-propelled particles are often neither symmetric nor overdamped yet underlie random fluctuations from their surroundings. Active Brownian motion has already been generalized to include asymmetric particles. Separately, recent findings have shown the importance of inertial effects for particles of macroscopic size or in low-friction environments. We aim to consolidate the previous findings into the general description of a self-propelled asymmetric particle with inertia. We derive the Langevin equation of such a particle as well as the corresponding Fokker-Planck equation. Furthermore, a formula is presented that allows to reconstruct the hydrodynamic resistance matrix of the particle by measuring its trajectory. Numerical solutions of the Langevin equation show that, independent of the particle's shape, the noise-free trajectory at zero temperature starts with an inertial transition phase and converges to a circular helix. We discuss this universal convergence with respect to the helical motion that many microorganisms exhibit.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – Project-ID 433682494 - SFB 1459

CPP 16.11 Tue 12:45 H18

Stochastic motion under active driving due to inverted dry (solid) friction — ●Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

It has become common to describe the motion of actively driven or self-propelled objects using a driving force of constant magnitude. We assume that this driving force always acts along the current velocity direction. Moreover, we consider objects featuring a nonpolar axis, along which driving and propagation occur [1].

In that case, spontaneous symmetry breaking decides on the heading of propagation, that is, “forward” or “backward” along the nonpolar axis. Stochastic effects may reverse the velocity and thus the direction of the driving force.

As it turns out, active driving under these circumstances corresponds to inverted dry (solid) friction of the Coulomb type. Corresponding tools of theoretical analysis can thus be adopted, mapping the velocity spectrum to the one of a quantum-mechanical harmonic oscillator subject to a repulsive delta potential. In this way, the diffusion coefficient can be calculated analytically. We evaluate velocity and displacement statistics. Outward propagating displacement maxima emerge under increased active driving. The trajectories feature pronounced cusps when velocity reversals occur.

Our results should apply, for instance, to certain types of vibrated nonpolar rods and swimming bacteria that may reverse their propagation direction.

[1] A. M. Menzel, submitted.

CPP 17: Poster 2

Topics: 2D Materials (17.1-17.3), Composites and Functional Polymer Hybrids (17.4-17.6), Crystallization, Nucleation and Self-Assembly (17.7-17.12), General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (17.13-17.15), Hydrogels and Microgels (17.16-17.21), Interfaces and Thin Films (17.22-17.31), Nanostructures, Nanostructuring and Nanosized Soft Matter (17.32-17.35), Polymer and Molecular Dynamics, Friction and Rheology (17.36-17.38), Polymer Networks and Elastomers (17.39-17.41).

Time: Tuesday 11:00–13:00 Location: P2

CPP 17.1 Tue 11:00 P2

Simulation of vapour flow through aperture arrays for quantifying gravimetric mass loss measurements — ●Riko Korzetz, Lennart Schulte, and André Beyer — Bielefeld University

Gravimetric mass loss measurements are frequently employed to investigate the permeative behaviour of 2D membranes with respect to vapours of different solvents. Due to constraints in these measurements, insufficient circulation causes the build-up of concentration gradients in the vapour phase, which is known as concentration polarization. This leads to a seemingly non-intuitive permeation behaviour, which complicates the evaluation of the measured data.

Here, we present finite-element simulations that were employed to investigate this effect with respect to different types of membrane supporting apertures and aperture arrays. Both open orifices as well as membranes with different permeance values have been modelled to achieve a quantitative understanding of the relevant effects in mass loss measurements.

We found that for open orifices and apertures with highly permeable membranes, the diffusion from the bulk towards the membrane is the rate-limiting step. This results, for example, in a linear dependence between the permeation rate and the edge length of single open orifices. On the other hand, a dependence on the free-standing area occurs in the case of membranes with a sufficiently low permeance. We devised a phenomenological model to describe the permeation rate in dependence of the membrane permeance as well as support geometry, which allows correction of these effects when evaluating such measured data.

CPP 17.2 Tue 11:00 P2

Preparation and characterization of photosensitive nanomembranes — ●Verena Müller[1], Maria Küllmer[1], Florian Küllmer[1,2], Hans-Dieter Arndt[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]Friedrich Schiller University Jena, Institute of Organic Chemistry and Macromolecular Chemistry, Humboldtstraße 10, 07743 Jena

Carbon nanomembranes (CNMs) are two-dimensional (2D) organic materials with a molecular thickness that are synthesized by low-energy electron irradiation of aromatic self-assembled monolayers (SAMs). Using the molecular design, CNMs can be prepared with tunable physical and chemical properties and employed on their own, e.g. as separation membranes or in combination with other 2D materials in hierarchically assembled van-der-Waals heterostructures. Here we present the engineering of photosensitive nanomembranes *via* post-functionalization of $\sim 1\,\mathrm{nm}$ thick amino-terminated CNMs with azobenzene molecules. We characterize their properties using surface science techniques including X-ray photoelectron spectroscopy (XPS) and compare the obtained characteristics with the azobenzene-based SAMs.

CPP 17.3 Tue 11:00 P2

Selective Diffusion of $\mathbf{CO_2}$ and $\mathbf{H_2O}$ through Carbon Nanomembranes in Aqueous Solution as Studied with Radioactive Tracers — Raphael Dalpke[1], Anna Dreyer[2], Riko Korzetz[1], ●Lennart Schulte[1], André Beyer[1], and Karl Josef Diez[2] — [1]Faculty of Physics, Bielefeld University — [2]Faculty of Biology, Bielefeld University

A well-known approach of improving membrane separation processes is the attempt to utilize 2D materials. In particular, carbon nanomembranes (CNMs) are promising candidates due to their extremely high areal pore density. Specifically, CNMs made from terphenylthiol (TPT) exhibit a very high water permeance while blocking ions as well as many gases and vapours. Here, we present permeation measurements of TPT-CNMs utilizing radioactive tracer molecules to characterize diffusion of $[^{3}\mathrm{H}]\mathrm{H_2O}$, $[^{14}\mathrm{C}]\mathrm{NaHCO_3}$, and $[^{32}\mathrm{P}]\mathrm{H_3\ PO_4}$ in aqueous solution. For full consideration of concentration polarization and outgassing effects a mathematical model was developed and verified using finite-element simulations. The experiment shows that water and carbonate can pass through the CNM while phosphate ions are completely blocked. Considering ion conductivity measurements, the obtained diffusion coefficients indicate that the permeation across the membrane primarily occurs by transport of neutral species.

CPP 17.4 Tue 11:00 P2

Dipolar Molecular Rotors in Surface-Anchored Metal Organic Frameworks — ●Xianghui Zhang[1], Sebastian Hamer[2], Ritesh Haldar[3], Daniel Reuter[4], Florian Paneff[1], Dirk Volkmer[4], Peter Lunkenheimer[4], André Beyer[1], Ian Howard[3], and Rainer Herges[2] — [1]Faculty of Physics, Bielefeld University, 33615 Bielefeld — [2]Otto-Diels-Institute for Organic Chemistry, Christian-Albrechts-University of Kiel, 24098 Kiel — [3]Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe — [4]Institute of Physics, Augsburg University, 86135 Augsburg, Germany

Molecular rotors arranged in the surface-anchored metal-organic frameworks (SURMOF) were investigated. The rotating part of each linker molecule consists of a fluorine-substituted phenyl group connected with acetylene linkages to the Cu clusters. Dielectric spectroscopy was used to investigate the rotation dynamics of molecular rotors in a parallel capacitor assembly. We determined an activation energy of 10 kJ/mol for one SURMOF type consisting of 3-[4-(2-carboxyethynyl)-2,3-difluoro-phenyl]prop-2-ynoic acid (C12H4F2O4) as dipolar linkers and 1,4-diazabicyclo(2.2.2)octane (DABCO) as pillars, at temperatures above 170 K. A smaller barrier of about 2 kJ/mol was found for the corresponding SURMOFs without any pillars. The analog made from the non-polar linker was used as a control system and showed no dielectric relaxation processes down to 20 K. The observed activation energy barriers are consistent with ab initio DFT modelling and classical dipole-dipole interaction calculations.

CPP 17.5 Tue 11:00 P2

Design, fabrication and nano-scale characterization of novel SEI layers — •Zhuijun Xu[1], Yanjun Cheng[2], Yonggao Xia[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Ningbo Institute of Materials Technology and Engineering, Chinese Academy of Sciences, 315201, Ningbo, China — [3]MLZ, TU München, 85748 Garching, Germany

Rechargeable lithium metal batteries have been recognized as one of the most promising energy storage devices due to their superior energy density. However, serious safety concerns and poor cyclability are challenges originating from an uncontrolled lithium dendrite growth and an unstable solid electrolyte interface (SEI) layer. One strategy to suppress dendrite growth is a surface modification with amphiphilic block copolymers, such as PDMS-b-PAA, which bear some clear advantages including absorbing mechanical stress, conducting lithium ion and controlling the lithium dendrite growth process. With ex-situ scattering techniques or in-situ scattering studies, the structures of the surface modified lithium metal anodes and structure formation processes are studied. In particular, by applying GISAXS, the horizontal structures and vertical structures of the polymer films on the lithium metal surfaces are investigated.

CPP 17.6 Tue 11:00 P2

In situ GISAXS printing of inorganic-organic hybrid nanostructures based on biopolymer templating — •Linus F. Huber[1], Stephan V. Roth[3], Kun Sun[1], Manuel A. Reus[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching — [3]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, 22607 Hamburg, Germany

Inorganic-organic hybrid nanostructures are interesting for the energy conversion through the thermoelectric effect. Thermoelectric generators based on abundant, environmentally friendly and affordable materials have historically had low effitiencies. The electrical conductivity, the Seebeck coefficient and the thermal conductivity need to be individually improved, to significantly enhance the thermoelectric figure of merit. Nanostructuring can improve these parameters and maximize the performance of thermoelectric materials. Beta-lactoglobulin is a bovine whey protein that is used as a template during sol-gel synthesis. Different titania thin film morphologies can be achieved by changing the pH-value and the beta-lactoglobuline concentration. To investigate the different titania morphologies, in situ GISAXS, GIWAXS and SEM are used. In situ GISAXS printing enables a time resolved investigation of the structure formation, domain sizes and domain distances. UV-Vis and Pl are used to analyze differences in the optical properties of the thin films. These structural and optical changes are then correlated with measurements of the Seebeck coefficient and the electrical conductivity.

CPP 17.7 Tue 11:00 P2

Two-step nucleation in confined geometry on a lattice gas model — •Jacob Holder, Ralf Schmid, and Peter Nielaba — Physics Department University of Konstanz, Konstanz, Germany

We deploy a degenerated Ising model to describe nucleation and crystallization from solution in a confined two-component system. The free energy is calculated using Metadynamics simulation. With nudged elastic band simulation we calculate the minimum energy path and give properties of the crystallization path. From the parameters and setup we find necessary conditions for the occurrence of two-step nucleation in our system.

CPP 17.8 Tue 11:00 P2

Nucleation patterns in polymer crystallization analyzed by machine learning — •Atmika Bhardwaj[1,2], Marco Werner[1], and Jens-Uwe Sommer[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e. V., Hohe Str. 6, Germany 01069 — [2]Technische Universität Dresden (TUD)

Today, many efforts seek to link machine learning (ML) algorithms to the concepts of theoretical physics. Our work focuses on developing ML tools to derive meaningful interpretations from the data generated through molecular dynamics simulations. We aim to find and quantify the nucleation patterns in polymer crystallization. The transition dynamics occurring under-cooled polymer melt is a local environmental phenomenon rather than a property of individual particles (or monomers), and depends on subtle conformation patterns such as entanglements between the chains. Our first objective is to define a set of fingerprint parameters to capture the crucial information in the local conformation and a monomer's environment and to quantify the degree of crystallinity. We use self-supervised auto-encoders to contain those local fingerprints. The second objective is to recognize the precursors or nucleation sites that stimulate crystal growth before the occurrence of such growth. We are currently working on both convolutional neural networks and recurrent neural networks to investigate the spatial and temporal patterns of the precursors.

CPP 17.9 Tue 11:00 P2

Laser control over crystallization and morphology of tetracene thin films — •Stefan Kowarik[1], Andika Asyuda[2], Linus Pithan[3], and Andreas Opitz[4] — [1]Physical Chemistry, University of Graz, Austria — [2]Institute for Physical Chemistry, Universität Heidelberg, Germany — [3]Institut für Angewandte Physik, Universität Tübingen, Germany — [4]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Nucleation and crystallization in thin-film growth are notoriously difficult to steer, but optical control offers exciting new possibilities for selecting specific polymorphic forms [1] or aligning the crystallite orientation in thin films [2]. Here we report an increase in crystallite size in vacuum-deposited tetracene thin films under illumination with a wavelength tuned to a specific absorption band of tetracene crystals. The morphological changes are induced with linearly and circularly polarized light and the larger crystallite size is accompanied by higher photoluminescence of tetracene. We propose a mechanism based on optical heating of specifically oriented crystals during growth, which leads to enhanced surface migration processes in these crystals and consequently larger crystals via Oswald ripening effects. The light-induced temperature effects are distinct from substrate heating both for linearly and circularly polarized light. Laser illumination, therefore, is a novel control parameter of growth and enables high crystallinity even for low substrate temperature deposition.

[1] L. Pithan, et al., Crystal Growth & Design 15.3 (2015): 1319-1324. [2] L. Pithan, et al., Advanced Materials 29.6 (2017): 1604382.

CPP 17.10 Tue 11:00 P2

Synthesis of Hard-Carbon Microspheres with Binary Size Distribution via Hydrothermal Carbonization of Trehalose — •Martin Wortmann[1], Waldemar Keil[2], Michael Westphal[1], Elise Diestelhorst[3], Jan Biedinger[1], Bennet Brockhagen[3], Günter Reiss[1], Claudia Schmidt[2], Klaus Sattler[4], and Natalie Frese[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Paderborn University, Paderborn, Germany — [3]Bielefeld University of Applied Sciences, Bielefeld, Germany — [4]University of Hawaii, Honolulu, USA

Hard Carbon microspheres (HCS) were synthesized via hydrothermal carbonization (HTC) of trehalose and subsequent pyrolytic post-carbonization at 1000°C. It was found that HTC of trehalose, in contrast to other saccharides, results in a distinctly binary sphere diameter distribution with monodisperse small spheres and polydispers large spheres. Pore formation, as visualized by charge-compensated helium ion microscopy, results in a strong increase in BET surface area. The chemical composition and crystallinity were examined before and after pyrolysis using a variety of spectroscopic methods. Strong compositional similarities were found to other saccharide-derived hydrochars, with a cross-linked furan-based polymer-structure before, and nano-crystalline carbon structure after pyrolysis. The binary size-distribution and large BET surface area make trehalose-derived HCS a highly promising material for applications in energy storage or catalysis.

CPP 17.11 Tue 11:00 P2

Physics of supersaturated, agitated sucrose solutions: Crystal nucleation and growth — •Hannah M. Hartge and Thomas

A. Vilgis — Max Planck Institute for Polymer Research, Mainz, Germany

Supersaturated sucrose solutions that have been sufficiently cooled without nucleation constitute a meta-stable system in which agitation promotes fast crystallization. Applications of this physically interesting process can be found for example in the production of fondant in confectionery. While just water and sucrose are present, the system goes through complex thermodynamic processes during crystallization, which are highly dependent on composition, temperature, and agitation.

In this work, we investigate how temperature and concentration affect nucleation, crystal growth and final particle size distribution of highly supersaturated sucrose solutions under agitation. To do so, the torque was measured during kneading of the samples at controlled temperature, followed by light microscopy and corresponding image analysis. When crystallization times were compared to classical nucleation theory, variations were found to be related to temperature and supersaturation in the same way as indicated by induction time models of statistical physics. Additionally, size distributions of the resulting crystal phases showed a strong dependence on temperature during agitation, sucrose content and according initial supersaturation.

CPP 17.12 Tue 11:00 P2

Following the directed self-assembly of crystallizable block co oligomers via in situ AFM — •Alexander Meinhardt and Thomas F. Keller — Centre for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Bottom up nanofabrication utilizing the molecular self-assembly of block co-oligomers with sub-10 nm domain sizes are widely discussed as a promising route for next generation photolithography. Double crystalline co-oligomers can be used to create well defined, high-fidelity nanostructures by controlling the competing driving forces microphase separation and crystallization. We report on the surface nanostructure formation and its temporal evolution during annealing of thin films of an amphiphilic double crystalline polyethylene-block-poly(ethylene oxide) co-oligomer (PE-b-PEO) on planar and patterned surfaces. Directing the self-assembly of such systems with physical or chemical guiding patterns can enable the formation of defined, large scale amphiphilic nanostructures, which could be of interest for various applications, e.g., biomaterials, photonics, and nanotechnology. However, there still remain several challenges regarding the characterization, defect density, pattern fidelity, and post processing of such block copolymer nanopatterns. By investigating the directed self-assembly (DSA) of the PE-b-PEO using AFM in situ, we aim to tune the balance of the involved driving forces and in turn create optimized nano-templates.

CPP 17.13 Tue 11:00 P2

Influence of the surface roughness and surface chemistry to understand slide electrification — •Benjamin Leibauer, Werner Steffen, and Hans-Jürgen Butt — Ackermannweg 10 55128 Mainz

In the last few years a lot of studies have shown that by contact electrification between water droplets and hydrophobic surfaces, it is possible to generate electricity in an environmentally friendly way.[1] The physical processes are still being discussed today and to extend the understanding Stetten et al.[2] have established an experimental setup that allows the drop charge of individual drops. In the work presented here we have studied with this setup the influence of the surface roughness and the chemistry of the substrates on hydrophobic to superhydrophobic substrates. We found that for the drop charge both parameters have an influence on at least the same order of magnitude.

[1] C. Wu, A. C. Wang, W. Ding, H. Guo, Z. L. Wang, Advanced Energy Materials 2019, 9, 1802906. [2] A. Z. Stetten, D. S. Golovko, S. A. Weber, H.-J. Butt, Soft Matter 2019, 15, 8667-8679.

CPP 17.14 Tue 11:00 P2

Dewetting dynamics and equilibrium droplet shapes for of visco-elastic substrates — •Khalil Remini[1], Leonie Schmeller[2], Dirk Peschka[2], Barbara Wagner[2], and Ralf Seemann[1] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Weierstrass-Institute, Berlin University, Berlin, Germany

In our study we are interested in the dewetting of liquid polymer layers (Polystyrene 18 kg/mol) with about 100 nm thickness from visco-elastic polydimethylsiloxane surfaces with elasticity ranging E = 1.2 MPa for Sylgard 184 to E = 3 kPa for Cy52-276. When heating the samples to temperatures where PS is liquid, holes nucleate in the initially uniform PS film. These holes grow during dewetting, coalesce and eventually form sessile droplets of a few micrometers in diameter sitting on the PDMS surface. Due to the particular situation of the adaptive PDMS substrate, we observe characteristic qualitative and quantitative differences in rim shapes, (dynamic) contact angles and dewetting velocities which are indicating differences in the underlying energy dissipation but might result also from potential phase separation of liquid and cross linked PDMS close to the three-phase contact line. To shed light on the impact of viscous and elastic properties and potential phase separation at the three phase contact line, we aim at a quantitative comparison of sessile (equilibrium) droplets on substrates having different elasticities and thus elastocapillary lengths.

CPP 17.15 Tue 11:00 P2

Messung von Kräften zwischen Tropfen und bewegten Oberflächen — •Marisa Fischer, Simon Schubotz, Jens-Uwe Sommer, Andreas Fery und Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Um einen Tropfen über eine Oberfläche zu bewegen, wird eine Kraft benötigt, die von deren Eigenschaften abhängt. Das zur Messung dieser Kraft entwickelte Drop Adhesion Force Instrument (DAFI) erlaubt die freie Wahl der Geschwindigkeit der Drei-Phasen Kontaktlinie und der Größe des Tropfens [1]. Die Kraftmessung erfolgt mittels des Hookschen Gesetzes, indem die Auslenkung einer im Tropfen befindlichen Glaskapillare gemessen wird.

Ein von der Bewegung des Tropfens aufgenommenes Video wird mit einem von uns entwickelten Analyseprogramm ausgewertet. Für die Übertragung größerer Kräfte wird ein Glasplättchen am Kapillarende befestigt, welches die Adhäsion zwischen Tropfen und Kapillare erhöht.

Mit dem entwickelten Aufbau wurden die Kräfte zwischen Wassertropfen und Polydimethylsiloxan (PDMS) sowie Poly(N-isopropylacrylamide) (PNiPAAm) Polymerbürsten untersucht. Dabei zeigte sich ein Zusammenhang zwischen dem Zustand der Oberfläche und der Kraft.

[1] D. W. Pilat u. a., Langmuir 2012, **28**, 49, 16812-16820

CPP 17.16 Tue 11:00 P2

In-situ Monitoring of Hard-Core Soft-Shell Microgels During Monolayer Drying — •Julian Ringling, Keumkyung Kuk, and Matthias Karg — Heinrich-Heine-Universität, Düsseldorf, Germany

Hard-core soft-shell (HCSS) microgels are interesting colloids with the potential to be used as model systems to understand crystallization and melting processes [1]. They spread at the air/water interface and self-assemble into 2D monolayers in which the cores do not touch directly due to shell-shell repulsion. Compression of such a monolayer allows control over the inter-particle distance by compressing the soft and deformable shell [2]. After transferring a compressed monolayer to a substrate, various structures can be observed [3]. Understanding and controlling the formation of those structures is essential for the use of the system as a model for crystallization.

Previously our group discovered a difference in monolayer structure at the air/water interface in comparison to the dried monolayer after transfer onto a substrate when using micron-sized silica-poly(N-isopropylacrylamide) HCSS microgels. To understand the phase transition/structural change occurring, we have monitored this phase transition/structural change using fluorescence and light microscopy. Here we present results from in-situ observations of drying 2D colloidal monolayers focussing on the effect of different parameters on drying and assembly behaviour.

[1] G. Wie et al., Soft Matter, 2013, 9, 9924-9930
[2] J. Tang et al., ACS Omega, 2018, 3, 12089 -12098
[3] S. Ciarella et al., Langmuir, 2021, 37, 5364-5375

CPP 17.17 Tue 11:00 P2

Investigation of Cononsolvency Phase Transition of Poly(sulfobetaine)-based Diblock Copolymer Thin Films — •Peixi Wang[1] and Peter Müller-Buschbaum[1,2] — [1]Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Lichtenbergstr. 1, 85748 Garching, Germany

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

CPP 17.18 Tue 11:00 P2

Core-shell microgels synthesized in continuous flow: Deep insight into shell growth by temperature-dependent FTIR spectrocopy — •Pascal Fandrich[1], Marco Annegarn[1], Lars Wiehemeier[1], Ina Ehring[1], Tilman Kottke[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, 33615 Bielefeld, Germany — [2]Biophysical Chemistry and Diagnostics, Bielefeld University, 33615 Bielefeld, Germany

While core-shell microgels have been intensively studied in their fully synthesized state, the formation mechanism of the shell growth has not been completely understood. Such insight is decisive for a customization of microgel properties for applications. In a novel approach, we synthesized microgels based on a N-isopropylmethacrylamide (NiPMAM) core and a N-n-propylacrylamide (NnPAM) shell in a continuous flow reactor. The shell growth is studied depending on the solution's time of residence inside the reactor. PCS experiments reveal a significant decrease of the volume phase transition temperatures of the core and the shell respectively, with increasing residence time. At early stages, a decreased swelling capacity is found before a discrete NnPAM shell is formed. Temperature-dependent FTIR spectroscopy shows that the decreased swelling capacity originates from a pronounced interpenetrated network between NnPAM and NiPMAM. AFM images resolve a raspberry-like structure after 3 min, pointing to an aggregation of NnPAM domains before the distinct shell forms.

CPP 17.19 Tue 11:00 P2

How ultrasound accelerates microgel adsorption kinetics — •Luca Mirau[1], Sebastian Stock[1], Amin Rahimzadeh[1], Sonja Wismath[2], Matthias Rutsch[2], Mario Kupnik[2], and Regine von Klitzing[1] — [1]Department of Physics, TU Darmstadt, Hochschulstr. 8, 64289 Darmstadt — [2]Measurement and Sensor Technology, TU Darmstadt, Merckstraße 25, 64283 Darmstadt

Poly-N-isopropylacrylamide (PNIPAM) based microgels (MGs) are surface-active and offer great opportunities as stabilizers of emulsions and foams. Due to their thermosensitive response, the MGs enable also destabilization on demand. However, emulsion formation implies energy input by stirring or ultrasonication. To understand this formation process, it is important to understand the interfacial adsorption of the MGs. A fast trigger to affect the adsorption process is given by ultrasonication. The present study shows the effect of ultrasound on the adsorption kinetics of PNIPAM MGs at the water-oil interface monitored by drop shape tensiometry. The adsorption kinetics of MGs accelerates with increasing ultrasonication intensity. The variation of different parameters, such as ultrasonic frequency, MG crosslinker density, concentration and phase composition, indicates that both acoustic streaming as well as ultrasound induced deswelling of MGs due to breakage of hydrogen bonding cause this acceleration.

CPP 17.20 Tue 11:00 P2

Interaction of soft microgel with solid silica particles at the air-water interface — •Carina Schneider, Sebastian Stock, Kevin Gräff, Franziska Jakob, and Regine von Klitzing — Departement of Physics, TU Darmstadt, Hochschulstraße 8, 64289, Darmstadt

Emulsions stabilized by multiple particle systems are interesting in various research fields, e. g., in the food industry or interfacial catalysis. The interaction of two or more nano-particle systems of different properties at liquid interfaces is important for the coalescence behavior of emulsion droplets stabilized by these particle mixtures. For instance, a mixture of hydrophilic microgel particles (MGs) and hydrophobic silica nano-particles (SiNP) is able to stabilize water in oil emulsions, which is not possible with MGs alone. Therefore, it is of special interest to understand the interaction of those particles at the interface. In this context, their lateral compression may simulate the droplet interfaces under coalescence conditions. For this purpose, we spread mixtures of poly-NIPAM MGs and spherical SiNPs at the air-water interface of a Langmuir trough and determined the compression isotherms. For deeper insights into the lateral structure formation, the particle layers were transferred onto Silicon wafers and scanned by atomic force microscopy. For low compressions, the elastic MG network dominates the isotherm while SiNP are situated between the MGs with low impact. For higher compressions, the inelastic SiNP structures are pushed onto the MGs and take over the resistance to the outer pressure.

CPP 17.21 Tue 11:00 P2

Adsorption kineticts of microgel particles at the air/water interface — •Kai Luca Spanheimer, Daniel Jäger, Sebastian Stock, and Regine von Klitzing — Department of Physics, TU Darmstadt, Hochschulstraße 8, 64289 Darmstadt

Interest in microgel particles (MGs) based on poly-N-isopropyl acrylamide (PNIPAM) as surface-active material remains high. The nano- to micrometer sized, cross-linked polymer particles are able to adsorb to water/air or water/oil interfaces spontaneously. Combined with their ability to act as carriers for drugs, recent studies showed, that they may act as transport vehicles for amphiphilic catalysts to the interface, resulting in improved interfacial catalysis, e. g., in Pickering emulsions. Despite much research on the interaction of MGs with various low and higher molecular weight material, the adsorption of MG/catalyst complexes at the interface is not yet well understood. In the presented work, the adsorption kinetics at the air/water interface is measured via change in surface tension over time by drop shape analysis. In order to disentangle different effects in case of MG/catalyst complexes the adsorption kinetics of pure MGs and mixtures of MGs with simple anionic and cationic surfactants as model systems for the catalysts is studied and compared with the adsorption of MG/catalysts complexes.

CPP 17.22 Tue 11:00 P2

A molecular dynamics approach to understand and control the catalyst enrichment at the IL/vacuum interface in SILP systems — Mattia Livraghi[1], Christian Wick[1,2], •David Matthew Smith[1,3], and Ana-Sunčana Smith[3] — [1]PULS Group, Institute for Theoretical Physics and Interdisciplinary Center for Nanostructured Films (IZNF), Friedrich-Alexander Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany — [2]Competence Unit for Scientific Computing (CSC), FAU, 91058 Erlangen, Germany — [3]Group of Computational Life Sciences, Division of Physical Chemistry, Ruder Bošković Institute, 10000 Zagreb, Croatia

Supported Ionic Liquid Phase Catalysis (SILP) improves the catalytic turnover by smearing a thin IL layer onto a support material, reducing the need for slow reactant transport inside viscous ILs. Next generation SILP technology will rely on confining the catalyst to the vacuum interface, spatially localising the chemical reaction. This will require a deep understanding of the interface enrichment and structuring of the individual chemical components. We investigated ionic liquids made of iodide and polyehtylene glycol imidazolium cations. Therefore, we parameterized atomic charges for the new ILs using multiple conformations during the RESP fitting procedure, compatible with the GAFF force field, and validated our simulations against experimental data. The (also newly parameterized) catalysts are Nickel(II) coordination compounds with task-specific carbene ligands. We investigate the influence of the structures of the ligands and the IL's chain on controlling the catalyst's distribution in and affinity for the IL-vacuum interface.

CPP 17.23 Tue 11:00 P2

Morphology control of titania thin films in a low temperature process — •Guangjiu Pan[1], Shanshan Yin[1], Nian Li[1], Tianfu Guan[1], Renjun Guo[1], Suzhe Liang[1], Yuqin Zou[1], Caroline Ehgartner[2], Nicola Hüsing[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materialchemie, Chemie und Physik der Materialien, Universität Salzburg, 5020 Salzburg, Austria — [3]MLZ, TU München, 85748 Garching, Germany

A low-temperature routine to realize inorganic electron-transport layers (ETLs) is important for the commercialization of perovskite solar cells. Fabricating ETLs at low temperature is energy saving and compatible with flexible substrates. In this work, titania thin films are synthesized at low temperature (below 100 Celsius degree) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-b-polyethylene oxide (PS-b-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). Tailoring titania film morphology in the low-temperature process is achieved by managing phase separation of the polymer template. The ratio of polymer, precursor, solvent, and catalyst for the sol-gel solution is varied to tune the thin film morphologies. The surface morphologies of titania films are probed via scanning electron microscopy and GISAXS. The optical properties of the films are examined with ultraviolet-visible spectroscopy.

CPP 17.24 Tue 11:00 P2

Soft Matter Food Physics: Oat Drink Foams — •Judith Hege, Antonia-Louisa Schlichting, Jana Reeh, and Thomas A. Vilgis — Max Planck Institute for Polymer Research, Mainz, Germany

For various applications, oat drink needs to provide a capacity to form stable, creamy, homogeneous foams. Such macroscopic foam properties are based on molecular interactions at the air-water interfaces and protein kinetics within the lamellae. However, the underlying structure-function relationships between molecular interactions and macroscopic foam properties are not yet fully understood, especially for multicomponent systems like plant-based drinks. Therefore, this study probed foams formed by an oat drink containing only water, oats, canola oil and salt.

Investigations focused on the influence of enzyme treatment, canola oil addition, heat treatment and homogenization parameters on foam properties. Accordingly, time-dependent foam height measurements were performed and supported by light microscopy, photography, and particle size measurements to compare the findings on the macroscopic scale with bubble size evolution and oil droplet distribution.

This study showed that protease treatment resulted in a higher foaming capacity, but lower foam stability and that heat treatment lessened the foam stability. Furthermore, addition of small contents of canola oil increased the foaming capacity, however, higher canola oil contents reduced foam stability. Furthermore, a longer duration and higher speed of homogenization treatment caused a more homogeneous emulsion and increased foaming capacity as well as foam stability.

CPP 17.25 Tue 11:00 P2

Spatial resolution of particle transport at interfaces — •Kevin Höllring[1], Andreas Baer[1], David M. Smith[2], and Ana-Sunčana Smith[1,2] — [1]PULS Group, FAU Erlangen-Nürnberg, Germany — [2]Group for Computational Life Sciences, Ruđer Bošković Institute, Zagreb, Croatia

Confined geometries play an important role in various applications, where it is generally important to be able to predict particle transport and mobility. Commonly used techniques like the Einstein-approach using the Mean Square Displacement (MSD) as well as Auto-correlation-function (ACF) related techniques rely on strong assumptions about spatial isotropy and homogeneity tied to conditions on local symmetry, that are not satisfied in these confined geometries, making it especially hard to resolve interface-orthogonal particle dynamics. Still other techniques like jump-diffusion are only able to approximate relative mobility and require calibration for each system.

We propose a theoretical model for resolving absolute interface-perpendicular diffusion based on the time particles spend within subspaces of confined systems that accurately predicts diffusion for simple point-like particles like water. In addition, we also present an extension to that model taking into account internal deformational degrees of freedom that can affect the observed particle lifetime.

By application of the proposed models to water as well as Imidazolium-based ionic liquids, we confirm their accuracy and versatility in the analysis of complex particle dynamics thus also proving their applicability to confined geometries.

CPP 17.26 Tue 11:00 P2

In-situ investigation during gold HiPIMS deposition onto polymers — •Yusuf Bulut[1,2], Kristian Reck[3], Matthias Schwartzkopf[1], Jonas Drewes[3], Suzhe Liang[2], Tianfu Guan[2], Thomas Strunkus[3], Franz Faupel[3], Peter Müller-Buschbaum[2,4], and Stephan V. Roth[1,5] — [1]DESY, 22607 Hamburg — [2]TU München, Physik Department, Lehrstuhl für Funktionelle Materialien, 85748 Garching — [3]CAU, Chair for Multicomponent Materials, Faculty of Engineering, 24143 Kiel — [4]MLZ, TU München, 85748 Garching — [5]KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE-100 44 Stockholm

Gold deposition via high power impulse magnetron sputtering (HiPIMS) allows to coat thin metal layers on heat sensitive materials such as polymers allowing for increased adhesion and density. HiPIMS allows deposition at a lower total deposited thermal energy in comparison to conventional magnetron sputtering, but this energy is delivered in a very short pulse exhibiting very high power and ionization. The consequences for the nucleation and growth processes during HiPIMS deposition are not sufficiently known. Therefore, we investigate the morphology evolution of thin gold layers on four polymer templates, namely polystyrene (PS), polyvinylalcohol (PVA), polystyrene sulfonicacid (PSS) and poly-4-vinylpyridin (P4VP). These polymers show different functional moieties and thus are expected to influence the growth of the gold layer. We present first results of our in situ investigations combining grazing-incidence small angle X-ray scattering (GISAXS), grazing incidence wide angle X ray scattering (GIWAXS).

CPP 17.27 Tue 11:00 P2

High-concentration Lithium-ion Electrolyte Overcomes the Challenges of High-temperature Lithium Batteries — •Tianle Zheng[1], Yajun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo, 315201, Zhejiang Province, P. R. China

Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. Herein, we demonstrate a new electrolyte that achieves an excellent stable long-term cycling at 100°C, well beyond the typical 60°C limits of normal conventional Li-ion batteries. The high concentrated lithium oxalyldifluoroborate (LiODFB) is selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte can promote to form a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells, and achieve reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) $>$ 99.3%. Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by molecular dynamics (MD) simulations and XPS characterization techniques, exploring a new way for future high-temperature electrolytes for Li-ion batteries.

CPP 17.28 Tue 11:00 P2

Sol-gel based tailored lithium-ion battery electrodes — •Ivana Pivarníková[1,2], Ralph Gilles[1], and Peter Müller-Buschbaum[1,2] — [1]MLZ, TU München, 85748 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Silicon based materials have been considered as one of the most promising candidates for the next-generation lithium-ion battery anodes, thanks to its low cost, non-toxicity and high theoretical gravimetric capacity (4200 mAh/g). One of the concepts for a suitable application is to design the mesoporous Si-based material via copolymer assisted sol-gel synthesis. 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 spin-coated onto the cleaned Si substrates and the removal of the template 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 the reaction compounds, choice of the deposition technique, choice of the final calcination step or choice of additives. The aim is to reach the desired thickness, porosity, conductivity and mechanical stability for a successful Li-ion battery anode application. The produced thin films are characterized by scanning electron microscopy (SEM), grazing incidence small-angle X-ray scattering (GISAXS), profilometry and ellipsometry measurements.

CPP 17.29 Tue 11:00 P2

Silicon-germanium based coating of anodes for Lithium-ion batteries — •Kexin Wu[1], Christian L. Weindl[1], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

Lithium-ion batteries (LIBs) have received increasing attention over several decades as an indispensable role in energy storage. The application of silicon anodes is hindered by their volumetric expansion after full lithiation, which causes collapse with three failure mechanisms including electrode pulverization, disconnection between the electrode and current collector, and continuous breaking and re-growth of the solid electrolyte interface (SEI) layer. To tackle this critical issue, the construction of hierarchical structures is a promising way to increase the stability of active materials. In our studies, Si/Ge hierarchical structures are built by chemical templating of pre-nanostructure self-assembled polystyrene nanoparticles, using an amphiphilic polystyrene-block-polyethylene oxide (PS-b-PEO) diblock copolymer as structure-directing agent. The diblock copolymers undergo microphase separation, which is further modified by solvent vapor annealing with dichloromethane (DCM) and SiCl4. By pyrolysis, mesoporous thin films are achieved. The desirable morphological and crystallographic studies are accomplished by GISAXS) SEM, AFM, and GIWAXS) The study is completed by galvanostatic cycling tests and impedance spectroscopy.

CPP 17.30 Tue 11:00 P2

Modeling of Nano-Porous Electrode Systems via Molecular Dynamics — •Philipp Stärk — SC Simtech, Uni Stuttgart, Germany

We use grand canonical Monte Carlo combined with atomistic-level MD to simulate open electrode systems at a constant potential. Using a multi-scale approach, our aim is to aid in the design of energy storage devices/electrocatalysis applications. In order to achieve this goal, we use different constant potential approaches to characterise the atomistic mechanisms behind charging and electro-catalytic product transport.

CPP 17.31 Tue 11:00 P2

Charging of dielectric surfaces in contact with aqueous electrolyte – the influence of CO_2 — •Peter Vogel[1], Nadir Möller[1], Pravash Bista[2], Stefan Weber[2], Hans-Jürgen Butt[2], Benno Liebchen[3], and Thomas Palberg[1] — [1]Institut für Physik, Johannes Gutenberg Universität, 55128 Mainz (Germany) — [2]Max Planck Institut für Polymerforschung, 55128 Mainz (Germany) — [3]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, 3 64289 Darmstadt (Germany)

The charge state of dielectric surfaces in aqueous environments is of fundamental and technological importance. We use super-heterodyne light scattering in a custom-made cell to study the influence of dissolved CO_2 on the charging of three, chemically different surfaces. We compare an ideal, CO_2-free reference state to ambient CO_2 conditions. Systems are conditioned under conductometric control at different low concentrations of NaCl. As expected for constant charge densities, ζ-potentials drop upon increasing the salt concentration in the reference state. Presence of CO_2 leads to an overall lowering of ζ-potentials. Moreover, for the inorganic dielectric, the salt dependent drop is significantly weakened, and it is inversed for the organic dielectrics. We suggest that at ambient conditions, the charge state of dielectric surfaces is related to dielectric charge regulation caused by the salt concentration dependent adsorption/desorption of CO_2.

CPP 17.32 Tue 11:00 P2

Characterization of Nd complexes and processing of photonic crystal structures — •Miriam Gerstel[1], Muhammad Shaharukh[1], Ingo Köhne[2], Paul Mertin[3], Rudolf Pietschnig[2], Bernd Witzigmann[3], Johann Peter Reithmaier[1], and Mohamed Benyoucef[1] — [1]Institute of Nanostructure Technologies and Analytics (INA) — [2]Institute of Chemistry — [3]Institute of Computational Electronics and Photonics, CINSaT, University of Kassel, Germany

Lanthanide (Ln) ions are unique for applications in lighting, sensing, and display technologies. In our approach, we investigate the potential of using Ln(III) complexes as attractive luminescent materials due to its characteristics of narrow emission bands and wide emission spectrum. Two different types of Nd(III) complexes are investigated: Nd complexes with phosphonate ligands with varying aromatic residues and complexes where the Nd ion is incorporated in a polyoctahedral silsesquioxane cage. Optical properties of Nd complexes are determined by photoluminescence (PL) spectroscopy, which reveals three emission bands of Nd(III) ions in the NIR region. To achieve a lowdensity molecular distribution on the sample surface, the complexes are dissolved in dichloromethane and drop-casted on a flat surface. For light enhancement, molecules will be immobilized on photonic crystal cavities (PhCs). The fabrication of PhCs by electron-beam lithography, inductively coupled plasma reactive ion etching and selective wet etching techniques is discussed. This work is supported by the state of Hesse in the frame of LOEWE priority project SMolBits.

CPP 17.33 Tue 11:00 P2

Fabrication of photonic crystals for integration of molecules — •Özlem Urcan[1], Ranbir Kaur[1], Muhammad Shaharukh[1], Ingo Köhne[2], Rudolf Pietschnig[2], Johann Peter Reithmaier[1], and Mohamed Benyoucef[1] — [1]Institute of Nanostructure Technologies and Analytics (INA), Kassel, Germany — [2]Institute of Chemistry, Kassel, Germany

The control of light-matter interaction is an enabling technique for many emerging quantum technology applications. Photonic crystals (PhCs) are of particular interest since they can confine light in small mode volumes producing a strong interaction between light and emitters located in or near the cavity. Emitters such as lanthanide (Ln) molecules offer the potential of scalable quantum systems due to their characteristic narrow linewidth and wide emission spectrum.

This work focuses on the fabrication of PhCs by electron-beam lithography, inductively coupled plasma reactive ion etching and selective wet etching techniques and investigating different process parameters influencing the quality of PhCs. The morphological and optical properties of PhCs are characterized by scanning electron microscopy and micro-photoluminescence spectroscopy. In order to enhance the light emission, Ln molecules will be immobilized on the processed PhC cavities.

This work is supported by the state of Hesse in the frame of LOEWE priority project SMolBits

CPP 17.34 Tue 11:00 P2

Propandehydrierungskatalysatoren mit den Eisen(III)oxid-Nanopartikeln — •Irina Belova — Moscow, Russia

Propylen ist ein sehr wichtiger Industrierohstoff, aber das Wachstum seiner Produktion hat mit dem Wachstum des Verbrauchs nicht Schritt gehalten. Das größte Potenzial im Bereich der Propylenherstellung haben die Reaktionen der direkten und oxidativen Dehydrierung von Propan. Wir haben versucht, einen Propan-Dehydrierungskatalysator als Eisen-Nanopartikeln auf Aluminiumoxid zu erhalten. Um Nanopartikel zu bilden, griffen wir auf die Bildung von Eisenkomplexen mit Phenanthrolin zurück. Bei der Reaktion der direkten Propandehydrierung gibt es bei diesen Katalysatoren eine geringe Selektivität. Dabei schreitet Cracken schreitet aktiv voran. Es gibt jedoch immer noch eine Propandehydrierung . Wir planen, mit Sauerstoff gemischtes Propan benutzen. Wir erwarten, dass die *milde* Oxidation von Propan mit Sauerstoff besser verläuft.

CPP 17.35 Tue 11:00 P2

Polydisperse curved polymer brushes — •Marios Giannakou and Friederike Schmid — University of Mainz

In the past, polymer brushes have been investigated in the monodisperse limit or in flat geometries. These circumstances however aren*t as experimentally relevant, as monodisperse brushes are difficult to construct and brushes are found in curved geometries most of the times. Here, we attempt to resolve this issue by extending the already established mean-field theory describing polymer brushes developed by Cates et.al.. We develop a numerical method that allows us to investigate cylindrical and spherical geometries for arbitrary polydispersities. We then explore the uniform, Schulz-Zimm and monodisperse polymer distributions, and comment on the results.

CPP 17.36 Tue 11:00 P2

Temperature-dependent conformation behavior of isolated Poly(3-hexylthiopene) chains — •Sanwardhini Pantawane and Stephan Gekle — Biofluid Simulation and Modeling Theoretische Physik VI Universität Bayreuth 95440 Bayreuth Germany

We use atomistic as well as coarse-grained molecular dynamics simulations to study the conformation of a single Poly(3-hexylthiopene) chain as function of temperature. We find that mainly bundle and toroid structures appear with bundles becoming more abundant for decreasing temperatures and even more after adding solvent (THF), leading to a prominent swelling of the molecular size at a temperature of about 220K. This swelling is in close agreement with the interpretation of recent spectroscopic experiments (Panzer et al. J Phys Chem Lett 8, 114 (2017)). We further relate the temperature dependence of P3HT to that of simple Lennard-Jones model polymers in vacuum.

CPP 17.37 Tue 11:00 P2

Dynamic Origin of the Entropic Force on a Semi-Confined Chain — •Rodrique Badr[1], Lama Tannoury[2], and Leonid Klushin[3] — [1]Johannes Gutenberg University, Mainz, Germany —

[2]Martin Luther University, Halle-Wittenberg, Germany — [3]American University of Beirut, Beirut, Lebanon

Thermodynamics predicts that the free energy of confinement

$$F = B\frac{L}{D}$$

for a chain confined in a tube with thin and thick walls is the same in both cases. This equivalence implies that the force acting to eject the chain from semi-confinement is also the same. Thermodynamics, however, does not explain the dynamical origin of the force, but one can understand the force as originating from contacts with the surface of the boundary. Intuition suggests that the thin boundary should amount to fewer contacts and thus lead to a smaller ejection force when compared to the case of a thick boundary. Using coarse-grained molecular dynamics (MD) simulations, we support and validate the thermodynamic prediction that the magnitude of the ejection force is the same for different thicknesses of the boundary.
The forces are also found to be in good agreement with the scaling laws predicted by the thermodynamic approach. Finally, the results from our MD simulations provide an explanation of the origin of this equivalence of entropic forces, through the analysis of the radial distribution of contributions from the boundary to the ejection force.

CPP 17.38 Tue 11:00 P2

Computational study of the rheology of nanoparticle-polymer composites — •Leon Hillmann, Niklas Blagojevic, and Marcus Müller — Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

Matrix-filler interactions in nanoparticle-polymer composites play a crucial role in the manufacturing process as well as the properties of the final material. Therefore, understanding the interplay between the parameters, such as shape, concentration, and size, is paramount for the design process of new composites. Computer simulations of these materials, however, pose several challenges due to the vast differences in the length scales involved, ranging from atomistic forces up to large-scale self-assembling structures. Here, a single nanoparticle embedded in polymer melt, represented by a highly coarse-grained, Gaussian, bead-spring model, is studied by dissipative particle dynamics (DPD) simulations. The nanoparticle-polymer interaction is adjusted with iterative Boltzmann inversion to match predictions of the density profile from atomistic simulations. Measurements of the nanoparticle's velocity autocorrelation function are then used to determine the memory kernel in a generalized Langevin equation. To what extent does the motion of the nanoparticle provide information about the viscoelastic properties of the surrounding melt? To this end, a numerical solution of the corresponding inverse problem is presented, which arises from a reformulation of the problem as the inversion of a triangular Toeplitz matrix. The results are finally compared with the predictions made by the Rouse model for unentangled polymer melts.

CPP 17.39 Tue 11:00 P2

Anomalous Diffusion of Diisocyanate in Cross-linked Silicone — •Martin Wortmann[1], Klaus Viertel[2], Natalie Frese[1], Waldemar Keil[3], Claudia Schmidt[3], and Bruno Hüsgen[2] — [1]Bielefeld University, Bielefeld, Germany — [2]Bielefeld University of Applied Sciences, Bielefeld, Germany — [3]Paderborn University, Paderborn, Germany

In industrial applications of polyurethane vacuum casting, silicone casting molds are used to replicate complex three-dimensional master patterns for prototypes and small series production. The undesired diffusion of isocyanate from the casting resin into the silicone causes gradual degradation of the casting molds. In this contribution, we present mathematical models for the anomalous diffusion process and a comprehensive description of the underlying chemical and physical mechanisms. The polymerization of the isocyanate with residual moisture to polyurea within the silicone matrix leads to a time dependence of both the surface concentration and the diffusion coefficient. The resulting concentration distribution over time and cross-section is modelled by analytical solutions to the diffusion equation.

CPP 17.40 Tue 11:00 P2

Molecular Dynamics Simulation of Free chain Diffusion into a Regular Network — •Jude Ann Vishnu[1] and Friederike Schmid[2] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Johannes Gutenberg University, Mainz, Germany

Thermo-sensitive hydrogels have attracted considerable attention in the field of bio chemistry and bio-medicine. Earlier works show that microfluidics can be used to create core-shell particle with decoupled elasticity and surface adhesiveness. However these experiments could not achieve proper control over the core-shell interconnectivity. We use MD simulations to understand and quantify the diffusive interpenetration of these shell polymers into a core gel. The simulation uses a Regular network to model the gel which is diffusively invaded via a polymer solution. We look into the interfacial profile and the ways to control this core-shell connectivity. The density profiles show a clear dependence of penetration on shell polymer concentrations. This is also seen in the degree of interfacial integration and diffusion depths. Finally the analysis of diffused free chain within the gel shows the emergence of large clusters leading to percolation.These results give us insight into how the factors like the core-shell polymer contact time, shell polymer concentration, etc can help us fine tune the core-shell connectivity in experiments.

CPP 17.41 Tue 11:00 P2

Nucleation of separating liquid phases in elastic polymer networks — •Charlotta Lorenz, Carla Fernández-Rico, and Eric Dufresne — Soft and Living Materials, ETH Zurich, Zurich, Switzerland

Arrested phase separation is a key mechanism used by living systems to create well-controlled nanostructures. One of the most salient examples is structural color as present in some bird and insect species. Besides fascinating optical properties, phase-separating composite systems can have astonishing mechanical properties: For example, liquid inclusions can stiffen polymer networks. These mechanical properties have been less studied compared to the optical properties. To study the mechanical properties we use a sample system of a polymer network made of PDMS and fluorinated oil. We aim to control mechanical properties by tuning the structure of the phase-separated domains. Structure of the phase separating domains can be influenced by their nucleation. We vary typical parameters which could determine the nucleation such as the mesh size of the polymer network and total liquid fraction. We employ small-angle X-ray scattering, tensile tests and indentation experiments to study nucleation and mechanical properties of phase-separating samples. Our studies can result in mechanically highly flexible, self-assembled materials, which are comparatively fast and easy to produce.

CPP 18: Complex Fluids and Colloids, Micelles and Vesicles (joint session CPP/DY)

Time: Tuesday 11:30–13:00 Location: H38

Invited Talk CPP 18.1 Tue 11:30 H38

How X-rays can reveal waters mysteries — •Katrin Amann-Winkel — Max-Planck-Institut für Polymerforschung, Mainz, Germany — Johannes Gutenberg Universität Mainz, Institut für Physik, Mainz, Germany — Stockholm University, Department of Physics, Stockholm, Sweden

Water is ubiquitous and the most important liquid for life on earth. Although the water molecule is seemingly simple, various macroscopic properties of water are most anomalous, such as the density maximum at 4°C or the divergence of the heat capacity upon cooling. Computer-simulations suggest that the anomalous behaviour of ambient and supercooled water could be explained by a two state model of water. An important role in this ongoing discussion plays the amorphous forms of water [1]. Since the discovery of two distinct amorphous states of ice with different density (high- and low density amorphous ice, HDA and LDA) it has been discussed whether and how this phenomenon of polyamorphism at high pressures is connected to the occurrence of two distinct liquid phases (HDL and LDL). X-ray scattering experiments on both supercooled water [2] and amorphous ice [3] are of major importance for our understanding of water. In my talk I will give an overview on our recent experiments on supercooled water and amorphous ices. [1] K. Amann-Winkel et al., Waters controversial glass transition, Rev. Mod. Phys. 88, (2016) [2] K.H. Kim, et al., SCIENCE 358, 1589 (2017) [3] K.H. Kim, et al., SCIENCE 370, 6519, 978 (2020)

CPP 18.2 Tue 12:00 H38

Electrostatic Shielding Behavior of Keggin Anions in Aqueous Solution — •Thomas Tilger 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.

Therefore, 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. Whilst this description provides a good agreement with experimental data for 1:1 electrolytes, larger deviations appear for systems of higher valency. For a detailed examination of the van der Waals and electrostatically dominated regimes, we directly measure the forces between colloidal silica particles in aqueous solutions by the colloidal probe AFM (atomic force microscopy) technique.

Varying the concentration of monovalent salts and acids allows us to demonstrate the transition from the double layer to the van der Waals dominated regime and to determine the pH dependence of the colloidal probes double layer potential. Similar measurements for phosphotungstic (PTA, a 1:3 system) and silicotungstic acid (STA, a 1:4 system) - both nanometer-sized anions of the Keggin type - can still be described with the DLVO theory, but reveal significant deviations between the calculated and measured ionic strengths.

CPP 18.3 Tue 12:15 H38

Influence of the imbibition of colloids through the morphology of porous CNF layers — •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], Calvin Brett[1,3], Jan Rubeck[1], Matthias Schwartzkopf[1], Eva Malmström[3], Daniel Söderberg[3], Peter Müller-Buschbaum[2,5], and Stephan V. Roth[1,3] — [1]DESY, 22607 Hamburg, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]KTH Royal Institute of Technology, 10044 Stockholm, Sweden — [4]Institute for X-ray Physics, Goettingen University, 37077 Goettingen, Germany — [5]MLZ, TU München, 85748 Garching, Germany

Functionalization of porous materials in terms of optical, chemical, and mechanical properties is readily achieved by applying colloidal layers. Our goal is to functionalize porous cellulose nanofibril (CNF) templates by applying tailored core-shell colloids with specific surface properties. The colloidal layer formation influencing the surface properties can be tuned by the deposition conditions and subsequent annealing. Therefore, we applied colloidal inks (poly(butyl methacrylate) and poly(sobrerol methacrylate) in aqueous dispersion) with different glass transition temperatures T_g as the colloidal layers on the CNF templates. During the deposition, the colloids partially enter the CNF layer to fill the CNF voids and remain on the CNF surface, leading to complex drying processes. The morphology of the mixed CNF / colloidal thin film changes when T_g of the colloids is exceeded.

CPP 18.4 Tue 12:30 H38

Elastic core-shell materials and their deformational behavior — Jannis Kolker[1], •Lukas Fischer[2], Andreas M. Menzel[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

Elastic materials consisting of an inner part, a core, and an outer part, a shell, of possibly different material properties can be found from planetary scales down to the colloidal microscale. We here describe a situation amenable to analytical theory, namely the linear elastic deformation of a spherical core-shell system in response to an equatorial load in form of a force line density [1]. The relevance of this setup lies in, e.g., functionalized microgel particles absorbed to fluid-fluid interfaces or macroscopic illustrative show-and-tell objects.

Situations of different elastic properties and sizes of core and shell are analyzed to study their influence on the deformational response of the whole system. For example, tuning the two Poisson ratios allows to adjust the relative degree of oblate or prolate deformations and change in volume between core and shell. Due to the overall spherical shape and the two-component structure, the stress and strain distributions become rather inhomogeneous. Using different core and shell materials in colloidal microgel particles allows for inner functionalization while simultaneously adjusting the outer wetting properties.

[1] J. Kolker, L. Fischer, A. M. Menzel, H. Löwen, *J. Elasticity*, in press.

CPP 18.5 Tue 12:45 H38

Effective Thomas-Fermi screening approach and wetting transition at charge/metal interfaces — •Alexander Schlaich[1,2], Dongliang Jin[1,3], Lyderic Bocquet[4], and Benoit Coasne[1] — [1]Univ. Grenoble Alpes, CNRS, LIPhy, Grenoble, France — [2]Stuttgart Center for Simulation Science, Universität Stuttgart, Germany — [3]Institut fur Theoretische Physik, Technische Universitat Wien, Austria — [4]Laboratoire de Physique de l'Ecole Normale Supérieure, CNRS, Université PSL, Sorbonne Université, Sorbonne Paris Cité, Paris, France

At the nanometer scale the commonly employed image charge approach to obtain the electrostatic interactions close to a metallic interface breaks down due to the finite screening in any real metal. We develop an effective approach that allows dealing with any real metal using the Thomas-Fermi formalism. [1]

We find a microscopic picture based on the Gibbs-Thomson equation for capillary freezing of an ionic liquid. An unprecedented wetting transition is found upon switching the confining medium from insulating to metallic. The wetting behavior at imperfect metals raises new challenging questions on the complex behavior of charged systems in the vicinity or confined within surfaces.

[1] A. Schlaich, D. Jin, L. Bocquet & B. Coasne, Nat. Mater. 1 (2021).

CPP 19: Perovskite and Photovoltaics 2

Time: Wednesday 9:30–11:00 Location: H38

Invited Talk CPP 19.1 Wed 9:30 H38

Elucidating the role of antisolvent polarity on the surface chemistry and optoelectronic properties of lead-halide perovskite nanocrystals — •Robert Hoye — Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom

Lead-halide perovskites (LHPs) have emerged as highly-promising contenders for light-emission applications, particularly in the form of nanocrystals (NCs), owing to their advantages of high photoluminescence quantum yield (PLQY), along with tunable, sharp emission peaks. Achieving high-quality NCs critically depends on the purification process, which often makes use of an antisolvent. Despite its important role, the mechanism by which the antisolvent influences the surface properties of the NCs is not well understood. In this talk, we examine the influence of the polarity of the antisolvent on the properties of the model NC system CsPbBrxI3-x. The antisolvents we compare are (in order of increasing polarity): methyl acetate, acetone and butanol. We find that as the polarity of the antisolvent increases, there is a greater blue-shift in the photoluminescence peak, owing to the removal of iodide. Through detailed nuclear magnetic resonance measurements, we find that this occurs due to more polar antisolvents having a higher propensity to induce a condensation reaction between the oleic acid and oleylamine ligands on the NCs, leading to their removal in the form of amides, which leads to the removal of surface iodides. This work shows that minimising surface damage to LHP NCs requires the selection of low polarity antisolvents.

CPP 19.2 Wed 10:00 H38

Simulation of the impact of processing conditions on the perovskite film morphology — •Martin Majewski, Olivier Ronsin, and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen- Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany

The solution-processed perovskite layer forms complex structures during drying. This morphology of the dry film heavily influences the efficiency of the final solar cell. The impact of the physical mechanisms on the morphology, like for example nucleation and evaporation rate, in a drying, crystallizing wet film is not really understood yet. Therefore a better understanding of the interplay of these phenomena is needed.

We will present phase field simulations which are capable to describe the main physical processes like: evaporation, diffusion, spontaneous nucleation, crystal growth and advection, to investigate the impact of processing conditions on the final morphology of the perovskite film. Comparisons of the simulation to the theory will be presented. First simulations of drying solutions, including all physical phenomena, will be shown and compared to experiments.

CPP 19.3 Wed 10:15 H38

Influence of crystallization on the structural and optical properties of lead-free Cs2AgBiBr6 perovskite crystals — •Melina Armer[1], Julian Höcker[2], Carsten Büchner[1], Sophie Häfele[1], Patrick Dörflinger[1], Maximilian T. Sirtl[3], Kristofer Tvingstedt[1], Thomas Bein[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ludwigs Maximilian University München, 80539 München — [3]Ludwigs Maximilian University München, 81377 München

As conventional perovskite solar cells contain lead and therefore suffer from toxicity issues, finding stable lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, lead-free Cs2AgBiBr6 single crystals have been synthesized by slowly evaporating organic solvents and by using the well-known controlled cooling technique. The evaluation of solubility curves showed that slow evaporation enables crystal growth in a wide range of temperatures. We further used the controlled cooling technique as a reference to the slow evaporation method to grow crystals at different temperatures. The quality of the synthesized crystals was characterized by X-ray diffraction (XRD) and energy dispersive X-ray (EDX) measurements. Furthermore, photoluminescence excitation (PLE) and absorption measurements were conducted to investigate the relationship between Urbach energy and the growth method and temperature. As a result, we found that growth temperatures significantly impact the amount of tail-states present in the perovskite crystals.

CPP 19.4 Wed 10:30 H38

Real-time texture and phase evolution tracking of the annealing process of slot-die coated perovskite by in situ GIWAXS — •Manuel A. Reus[1], Lennart K. Reb[1], Alexander F. Weinzierl[1], Christian L. Weindl[1], Renjun Guo[1], Tianxiao Xiao[1], Matthias Schwartzkopf[2], Andrei Chumakov[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]MLZ, TU München, 85748 Garching

In perovskite solar cell material research the thin-film morphology determines the quality of the absorber material and consequently device performance. To scale up material deposition towards, e.g., roll-toroll compatible techniques, the influence of the deposition method on morphology needs to be known to control the process. Here, we apply in situ grazing-incidence wide-angle x-ray scattering (GIWAXS) on the annealing process of slot-die coated lead iodide and slot-die coated methylammonium iodide, that react to perovskite under heat. We track the conversion in real-time and extract relevant parameters concerning texture and phase evolution. As a reference, we show GIWAXS data of spin-cast equivalent systems and show the resulting morphology and kinetics differences traced back to the deposition method.

CPP 19.5 Wed 10:45 H38

Temperature-reduced and rapid growth of hybrid perovskite single crystals — •Julian Höcker[1,2], Felix Brust[1], Melina Armer[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Experimental Physics - Soft Condensed Matter, Ludwig Maximilian University of Munich, 80539 Munich, Germany

Organolead trihalide perovskite single crystals are gaining more and more interest in the field of semiconductor research since they can be used for a variety of technical applications, like photodetectors or solar cells. To date, exclusively solution-processed perovskite crystals have been used for the fabrication of such device prototypes. A supersaturated perovskite solution is caused either by a temperature change, solvent evaporation, chemical reaction, or a combination of the methods. The aim of the various processes is to achieve rapid growth of crystals with controlled structure, size, shape, and yield. In addition, the crystalline components must exhibit high physical and chemical qualities to be applied as semiconducting components. However, these high requirements and numerous criteria cannot always be fully met by standard techniques like inverse temperature crystallisation. In order to grow large-sized OLTP single crystals in a controlled and simple manner from solution in the shortest possible time, we developed a crystallisation process based on primary alcohols. As a result, the blends based on perovskite precursor solution and alcohols lead to a significant reduction in their retrograde solubility and enable a temperature-reduced crystallisation pathway to grow single crystals.

CPP 20: General Session to the Symposium: Interplay of Substrate Adaptivity and Wetting Dynamics from Soft Matter to Biology (joint session CPP/DY)

Time: Wednesday 9:30–11:15 Location: H39

CPP 20.1 Wed 9:30 H39

Adaptive two capacitor model to describe slide electrification in moving water drops — •Pravash Bista[1], Amy Z. Stetten[1], William S.Y Wong[1], Hans-Jürgen Butt[1], and Stefan A.L. Weber[1,2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Johannes Gutenberg University, Department of Physics, Staudingerweg 10, 55128 Mainz, Germany

Slide electrification is a contact-charge separation where neutral water drops slide over a neutral hydrophobic surface, accumulating and leaving behind a net charge. The accumulated drop charge for successive sliding drops decreases and eventually reaches a steady state. On hydrophobic and hydrophilic mixed surfaces, even a polarity flipping of drop charge depending on a drop rate was observed. Here, we describe this effect in terms of a voltage generated at the three-phase contact line. This voltage moves charges between capacitors, one formed by the drop combined with the solid surface and one on the solid-surface. By introducing an adaptation of the voltage upon water contact, we can model drop charge experiments on different surfaces, including more exotic ones with drop-rate-dependent charge polarity. Thus, the adaptive two capacitor model enables new insights into the molecular details of the charge separation mechanism.

CPP 20.2 Wed 9:45 H39

Memory effects of PNiPAAm brushes in different atmospheres — •Simon Schubotz, Marisa Fischer, Jens-Uwe Sommer, Petra Uhlmann, Andreas Fery, and Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany

Some polymer brushes show a co-nonsolvency effect: They collapse in a mixture of two good solvents at some specific mixing ratio. In contrast to previous studies we concentrate on partial wetting of co-nonsolvent polymer brushes, i.e., on the dynamics of a three-phase contact line moving over such brushes.

We found that Poly(N-isopropylacrylamide) (PNiPAAm) brushes experiences a memory effect when consecutively depositing drops at the same position. Previously deposited drops adapt the brush and changes the wetting behavior (advancing contact angle) of subsequent drops.

We measure water drops in an ethanol-saturated atmosphere on PNiPAAm brushes. The measurements show that the memory effect is strongly effected by an ethanol-enriched atmosphere. At the three-phase contact line, due to evaporation from the drop, the composition of the atmosphere and probably also the brush will transition from an ethanol-rich state to a water-enriched state. Thus, the brush might pass through the co-nonsolvency regime. On large time scales the ethanol enriched gas phase and the water drop will become mixtures of ethanol and water. We present strategies to counter this mixing effect.

CPP 20.3 Wed 10:00 H39

Fast contact lines on soft solids — •Hansol Jeon[1,2] and Stefan Karpitschka[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany — [2]Georg-August-Universität Göttingen, Göttingen, Germany

When a droplet is resting on a soft surface, the capillary forces deform the surface into a sharp wetting ridge. The amplitude of the wetting ridge is determined by elasto-capillary length, but the angles by which the interfaces meet at the ridge tip only depend on the balance of surface tensions, the so-called Neumann balance. For moving contact lines, dissipation in the wetting ridge leads to viscoelastic braking. In recent literature, various effects that could alter Neumann balance and viscoelastic braking have been suggested, ranging from free, extractable oligomers to point forces emerg-ing from bulk viscoelasticity. We visualize moving wetting ridges at high spatio-temporal resolution and determine the tip geometry for various liquids and PDMS substrates. We observe an increase of the ridge opening angle at large speeds, even for very mild deformations caused by the low surface tension of a fluorinated oil. We also find no significant change in ridge rotation and opening angle for gels with different fractions of cross-linked and free chains, nor for different bulk rheological properties. These findings highlight the need for a non-trivial surface constitutional relation that is different from the bulk.

CPP 20.4 Wed 10:15 H39

Mixed grafted homopolymer and diblock copolymer functional brush layers upon humidity alterations: nanoscale morphology and transformations — •Apostolos Vagias[1], Theodore Manouras[2], Eleftherios Koufakis[2,3], Peixi Wang[4], Marcell Wolf[1], Fabian A. C. Apfelbeck[4], Sigrid Bernstorff[5], Maria Vamvakaki[2,3], and Peter Müller-Buschbaum[1,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [2]Foundation for Research and Technology (F.O.R.T.H.) Hellas, Institute of Electronic Structure and Laser,700 13 Heraklion, Crete, Greece — [3]Department of Materials Science and Technology, University of Crete, 700 13 Heraklion, Crete, Greece — [4]Physik-Department, Lehrstuhl für Funktionelle Materialien, Technische Universität München, 85748 Garching, Germany — [5]Elettra Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Using in situ grazing-incident small-angle X-ray scattering (GISAXS) measurements during water vapor uptake, we study the nanostructure morphology in the dry state, during vapor swelling and in the fully swollen state, for thin (<100nm) films of poly(2-(dimethylamino)ethyl methacrylate) (PDMAEMA) and poly(fluoroalkyl methacrylate) (POFPMA) homopolymer and PDMAEMA-b-POFPMA block copolymer dual functional, bactericidal and antifouling, brushes. Our surface energy and swelling studies, stress on the role alkyl chain length, charged groups and brush topology in morphology, for the brush functionality.

CPP 20.5 Wed 10:30 H39

Steering droplets on substrates with periodic wettability patterns and deformations — •Josua Grawitter and Holger Stark — Technische Universität Berlin, Institut für Theoretische Physik, Straße des 17. Juni 135, 10623 Berlin

Droplets are set in motion on substrates with a spatio-temporal wettability pattern as generated, for example, on light-switchable surfaces. To study such cases, we implement the boundary-element method to solve the governing Stokes equations for the fluid flow field inside and on the surface of a droplet and supplement it by the Cox*Voinov law for the dynamics of the contact line. Our approach reproduces the relaxation of an axisymmetric droplet in experiments, which we initiate by instantaneously switching the uniform wettability of a substrate quantified by the equilibrium contact angle.

First, we investigate a droplet on substrates with planar-wave-like wettability profile by varying the speed an wave length of the pattern. When the profile moves slowly, it moves the droplet moves steadily forward. Above a critical pattern speed the droplet performs steady oscillations, the effective (time-averaged) velocity of which decreases with the square of the pattern speed.

Second, we investigate a droplet on substrates which deform periodically according to a planar-wave profile. We analyze the effective velocity again as a function of wave speed and length and investigate specifically the influence of curvature changes on droplet motion.

CPP 20.6 Wed 10:45 H39

Spontaneous charging affects the motion of sliding drops — Xiaomei Li[1], Pravash Bista[1], Rüdiger Berger[1], Steffen Hardt[2], Holger Marschall[3], Hans-Jürgen Butt[1], and •Stefan A.L. Weber[1,4] — [1]MPI for Polymer Research, Ackermannweg 10, Mainz, Germany — [2]Institute for Nano- and Microfluidics, Technische Universität Darmstadt, Darmstadt, Germany — [3]Computational Multiphase Flows, Technische Universität Darmstadt, Darmstadt, Germany — [4]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

The motion of water drops on surfaces is still far from being fully understood. Previous understanding is that drop motion is dictated by viscous dissipation and activated dynamics at the contact line. To accurately measure the forces experienced by moving drops, we imaged their trajectory when sliding down a tilted surface, and applied the relevant equations of motion [1]. We found that drop motion on low-permittivity substrates is substantially influenced by electrostatic forces. Our findings confirm that electrostatics must be taken into consideration for the description of the motion of water, aqueous electrolytes and ethylene glycol on hydrophobic surfaces. Our results are relevant for improving the control of drop motion in many applications, including printing, microfluidics, water management and triboelectric nanogenerators. [1] Li, X. et al. Spontaneous charging affects the motion of sliding drops. Nat. Phys. (2022).

CPP 20.7 Wed 11:00 H39

Dynamic mesoscopic model for two-component compound drops — •Jan Diekmann and Uwe Thiele — Westfälische Wilhelms-Universität, Münster, Deutschland

We consider a mesoscopic model for two immiscible fluids forming two-layer liquid films or compound drops on a rigid solid substrate. The earlier macroscale description [1,2] is connected to our mesoscopic approach (building on [3]) via consistency conditions. Thereby we relate macroscale and mesoscale versions of the Young and Neumann relations at the liquid 1/solid/gas and liquid 1/liquid 2/gas contact lines, respectively. Furthermore, we employ the mesoscale model to investigate selected dewetting and coarsening processes for physically realistic parameters. The steady compound drops emerging from the time simulations are related to bifurcation scenarios determined via macroscale and mesoscale descriptions.

[1] L. Mahadevan, M. Adda-Bedia, and Y. Pomeau. "Four-phase merging in sessile compound drops". In: J. Fluid Mech. 451 (2002), pp. 411-420. [2] M. J. Neeson et al. "Compound sessile drops". In: Soft Matter 8 (2012), pp. 11042-11050. doi: 10.1039/c2sm26637g. [3] A. Pototsky et al. "Morphology changes in the evolution of liquid two-layer films". In: J. Chem. Phys. 122 (2005), p. 224711. doi: 10.1063/1.1927512. [4] Uwe Thiele et al. "Equilibrium contact angle and adsorption layer properties with surfactants". In: Langmuir 34.24 (2018), pp. 7210-7221.

CPP 21: Materials for Energy Storage (joint session KFM/CPP)

Chair: Prof. Dr. Theo Scherer (KIT, Karlsruhe)

Time: Wednesday 9:30–12:05 Location: H7

CPP 21.1 Wed 9:30 H7

Hybrid CuCo2O4 nanosheets as binder-free supercapacitor electrodes — •Zidong Wang[1,2], Yude Wang[2], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials and Energy, Yunnan University, 6500504 Kunming, Peoples Republic of China

CuCo2O4 is one kind of pseudocapacitive materials and it has a high theoretical capacitance, but it suffers from poor electrical conductivity. In this work, CuCo2O4 nanosheets were directly grown on a conductive skeleton to significantly enhance the conductivity and at the same time reduce the agglomeration of CuCo2O4 nanosheets. In addition, the hybrid nanosheet structures also expand the interface and provide more active electrochemical sites, facilitating kinetic processes and electrochemical reactions. The as-prepared CuCo2O4 nanosheets on a conductive skeleton were studied as binder-free electrode and exhibited outstanding electrochemical performance with the specific capacitance of 1595 F g*1 at a current density of 1 A g*1 and 85.1% capacitance retention after 4600 cycles. These results indicated that hybrid CuCo2O4 nanosheets has great application potential as binder-free electrode in supercapacitors.

CPP 21.2 Wed 9:50 H7

Investigation of K-ion Intercalation and Conversion in Layer Transiton Metal Disulfide anode: The case of MoS2 and WS2 — •Yulian Dong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) have a unique layered structure characterized by weak interlayer van der Waals interaction and strong in-plane covalent bonding. The structure allows the intercalation of guest species in the interlayer space, which shows impressive properties in potassium-ion batteries (PIBs). Thus, various 2D TMDs, including sulfides (MoS2, SnS2, WS2) and selenide (MoSe2 and VSe2), have been studied as potential anode materials for PIBs. This work compares the intercalation and conversion of K in MoS2 and WS2. Intercalation and conversion process is observed during potassium in MoS2 in a voltage range of 3.0-0.5V and 0.5-0.01V, respectively. By controlling cut-off voltage, the investigation demonstrated high capacities derived from the conversion, but it destroys the 2D diffusion pathways leading to an unstable cycling span. While the K+ storage in WS2 is governed by the intercalation reaction rather than the conversion reaction. It exhibited a low capacity decay rate at both low and high current densities as well as great rate capability.

CPP 21.3 Wed 10:10 H7

Elucidation of the Pore Formation Mechanism in Hard-Carbon Microspheres — •Martin Wortmann[1], Waldemar Keil[2], Michael Westphal[1], Elise Diestelhorst[3], Jan Biedinger[1], Bennet Brockhagen[3], Günter Reiss[1], Claudia Schmidt[2], Klaus Sattler[4], and Natalie Frese[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Paderborn University, Paderborn, Germany — [3]Bielefeld University of Applied Sciences, Bielefeld, Germany — [4]University of Hawaii, Honolulu, USA

Micro-spherical hydrochar can be carbonized by pyrolysis to produce hard-carbon microspheres with excellent electrochemical properties for the application as anode material in batteries. In this contribution, a temperature-resolved study of the chemical and morphological evolution of saccharide-derived hydrochar during pyrolysis up to 1000°C is presented. By combining a wide range of characterization methods all aspects of the structural transition are examined. The chemical processes occurring both in the bulk and at the surface of the carbon spheres are shown to affect the transition from an amorphous-polymeric to a nanocrystalline carbon-structure. The study focuses on the pore formation mechanism, which is driven by the aggregation of nanometer-sized oxygen-rich clusters at the sphere surface, which disintegrate in a narrow temperature range, leaving behind a mesoporous structure. The revealed molecular mechanisms provide key insights into the pyrolysis of carbonaceous materials.

CPP 21.4 Wed 10:30 H7

Hydrogenation of Pd nanoparticles at the nanoscale with in-situ TEM — •Svetlana Korneychuk[1,2], Stefan Wagner[1], Georgian Melinte[2], Darius Rohleder[3], Philipp Vana[3], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]INT, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Institute of Physical Chemistry Georg-August-University Göttingen, Göttingen, Germany

Palladium-based nanomaterials play an important role in hydrogen technology. Extreme affinity of palladium to hydrogen is very attractive for various applications. Besides catalysis, Pd nanoparticles can assist in hydrogen delivery into other materials for hydrogen storage through a spill-over process. Pd-based materials are also used as hydrogen purification membranes and hydrogen detectors. The hydrogenation and dehydrogenation process of Pd nanoparticles is hence of high interest in the applications mentioned above. Nanoscale systems reveal significant thermodynamic deviations from the bulk due to higher surface to volume ratio, absence of grain boundaries, different behavior of defects and mechanical stress. In this work, we investigate the behavior of Pd nanoparticles and formation of PdHx in real time with in-situ H2-gas TEM. Many applications require operation at elevated temperatures. With the special gas holder from Protochips it is possible to reach pressures up to 1 atmosphere and study the particles at elevated temperatures with the limit of 1000°C. We can observe the local phase change at different temperatures and pressures with the help of spectroscopic and diffraction techniques at the nanoscale.

15 min. break

CPP 21.5 Wed 11:05 H7

Mild-temperature solution-assisted encapsulation of phosphorus into ZIF-8 derived porous carbon as lithium-ion battery anode — •Chengzhan Yan[1], Shun Wang[2], and Yong Lei[1]

— [1]Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Key Laboratory of Carbon Materials of Zhejiang Province, Institute of Materials and Industrial Technologies, Wenzhou University, Wenzhou, Zhejiang, 325027, China.

The high theoretical capacity of red phosphorus (RP) makes it a promising anode material for lithium-ion batteries (LIBs). However, the large volume change of RP during charging/discharging imposes an adverse effect on the cyclability, and the rate performance suffers from its low conductivity. Herein, a facile solution-based strategy is proposed to incorporate phosphorus into the pores of MOF-derived carbon hosts under a mild temperature. With this method, the blocky RP is etched into the form of polyphosphides anions (PP, mainly P5-), making it easily diffuse into the pores of porous carbon hosts. Especially, the indelible crystalline surface phosphorus could be effectively avoided, which is generated in the conventional vapor condensation encapsulation method. Moreover, highly-conductive ZIF-8 derived carbon hosts with any pore smaller than 3 nm are efficient for loading PP and these pores can well alleviate the volume change. Finally, the composite of phosphorus encapsulated into ZIF-8 derived porous carbon exhibits a significantly improved electrochemical performance as LIBs anode.

CPP 21.6 Wed 11:25 H7

Study on Li Ion Diffusion in $\mathbf{Li_xV_2O_5}$ using First Principle Calculations and Kinetic Monte Carlo Simulations — •Fabian Dietrich[1], Eduardo Cisternas[1], Marcelo Pasinetti[2], and Gonzalo Dos Santos[2,3] — [1]Universidad de La Frontera, Temuco, Chile — [2]Universidad Nacional de San Luis, CONICET, San Luis, Argentina — [3]Universidad de Mendoza, Mendoza, Argentina

We study the Li diffusion in $Li_xV_2O_5$ $(0 < x \leq 1)$ - a potential cathode material for Lithium ion batteries. Different diffusion pathways in this material in dependence on the Li ion concentration are investigated by applying first-principles calculations. The results are used to obtain the corresponding diffusion coefficients by employing two complementary methodologies: Kinetic Monte Carlo (KMC) simulations and a statistical thermodynamics approach. The KMC simulations for two different crystal planes give new evidence that the diffusion occurs mainly along the [010] direction, while the corresponding diffusion coefficients show a temperature dependence obeying the Arrhenius' Law. The necessity of the consideration of concentration-dependent barrier heights in the KMC simulations are demonstrated by looking at the significant changes of the concentration-dependence of the diffusion coefficients. The simulated diffusion coefficients of the combined approach show a good quantitative agreement with experimental data reported previously.

CPP 21.7 Wed 11:45 H7

NMR studies of sintering effects on the lithium ion dynamics in $\mathbf{Li_{1.5}Al_{0.5}Ti_{1.5}(PO_4)_3}$ — •Philipp Seipel[1], Edda Winter[1], Michael Vogel[1], Tatiana Zinkevich[2], Sylvio Indris[2], Bambar Davassuren[3], and Frank Tietz[3] — [1]AG Vogel, Institute for Condensed Matter Physics, Technische Universität Darmstadt, Germany — [2]Karlsruhe Institut of Technology, IAM-ESS, Karlsruhe, Germany — [3]Forschungszentrum Jülich GmbH, IEK-1, Jülich, Germany

Various NMR methods are combined to study the structure and dynamics of $Li_{1.5}Al_{0.5}Ti_{1.5}(PO_4)_3$ samples, which were obtained from sintering at various temperatures between 650 °C and 900 °C and show high bulk conductivities up to 5 mS/cm. We use ^{7}Li NMR to study the transport mechanism in these glass ceramics [1]. Analysis of ^{7}Li spin-lattice relaxation and line-shape changes indicates the existence of two species of lithium ions with clearly distinguishable jump dynamics, which can be attributed to crystalline and amorphous sample regions. An increase of the sintering temperature leads to higher fractions of the fast lithium species with respect to the slow one, but hardly affects the jump dynamics in either of the phases. ^{7}Li field-gradient diffusometry reveals that the long-range ion migration is limited by the sample regions featuring slow transport. The high spatial resolution available from the high static field gradients of our setup allows us to observe also the lithium ion diffusion inside the small (< 100 nm) LATP crystallites, yielding a high self-diffusion coefficient of $D=2 \times 10^{-12}$ m^2/s at room temperature. [1]Winter et al., ZPCH, DOI:10.1515/zpch-2021-3109

CPP 22: Active Matter 3 (joint session BP/CPP/DY)

Time: Wednesday 9:30–12:30 Location: H16

CPP 22.1 Wed 9:30 H16

Collective foraging of microrobots trained by reinforcement learning — •Robert C. Löffler[1], Emanuele Panizon[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Quantitative Life Science, International Centre for Theoretical Physics, Trieste, Italy

From bacteria to mammals, collective behavior can be observed on all scales in nature. It is generally driven by the benefit to individuals when cooperating with others. However, the exact motivation of individuals to participate is challenging to investigate, as biological creatures are complex systems theirself. At the same time engineers seek to create collective groups of autonomous systems to perform dedicated tasks by cooperation.

Here we present an experimental model system of feedback-controlled microswimmers which are trained with multi agent reinforcement learning in an actor-critic scheme. A group of active particles is situated in a 2D environment containing a virtual food source which is changing position over time. Despite being rewarded individually for being inside the food source, particles show cohesive collective motion forming flocks and swirls. This is driven by the benefit of social information and collision avoidance, resulting in faster migration to a relocated food source. Understanding those mechanisms behind the emergence of collective behavior is of biological interest as well as to understand human crowd behavior and to design future robotic systems.

CPP 22.2 Wed 9:45 H16

Collective response of microrobotic swarms to external threats — •Chun-Jen Chen[1] and Clemens Bechinger[1,2] — [1]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [2]Centre for the Advanced Study of Collective Behaviour, Universität Konstanz, 78464 Konstanz, Germany

Many animal species organize within groups to achieve advantages compared to being isolated. Such advantages can be found e.g. in collective responses which are less prone to individual failures or noise and thus provide better group performance. Inspired by social animals, here we demonstrate with a swarm of microrobots made from programmable active colloidal particles (APs) that their escape from a hazardous area can originate from a cooperative group formation. As a consequence, the escape efficiency remains almost unchanged even when half of the APs are not responding to the threat. Our results not only confirm that incomplete or missing individual information in robotic swarms can be compensated by other group members but also suggest strategies to increase the responsiveness and fault-tolerance of robotic swarms when performing tasks in complex environments.

CPP 22.3 Wed 10:00 H16

Soft robots powered by magnetically driven active particles — •Hongri Gu and Clemens Bechinger — Fachbereich Physik, University of Konstanz, Germany

Active matter describes systems of a large number of self-driving particles that convert surrounding energy into active motion. Many of the emergent behaviors resemble life-like behaviors in nature. However, it is still unclear how one can utilize such active collective motions for engineering and robotic applications. In this talk, we would like to bridge the research fields of active matter and soft robots by designing soft machines powered by active matter. The main objective is to investigate the general interactions between swarm active particles and soft structures and use this knowledge to design a new type of soft robots that are driven by swarm active particles. To facilitate the investigation, we built a highly customizable fabrication process for magnetic composite soft structures at mesoscales based on two-step micromolding. We also built a modular magnetic actuation system based on rotating permanent magnets. This new experimental platform has an enormous design space for magnetic soft matters with the capability to tune individual system parameters. By carefully designing these parameters, it is possible to precisely tune the local magnetic, elastic, and hydrodynamic interactions between active particles and soft structures. This new type of soft machine can potentially take advantage of the robust dynamic states of the active matter, which can recover their functions from extreme mechanical deformations.

CPP 22.4 Wed 10:15 H16

Microswimmers in viscosity gradients — •Sebastian Ziegler[1], Maxime Hubert[1], and Ana-Sunčana Smith[1,2] — [1]PULS Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Division of Physical Chemistry, Ruder Bošković Institute Zagreb, Croatia

Regions of variant viscosity are ubiquitous in both inanimate systems as well as in living systems. It is therefore of great interest to understand the effect of viscosity gradients on the mobility of both passive particles as well as on active systems. We firstly study a system of passive spheres and provide a general expression for the asymptotic mobility matrix in small viscosity gradients. We apply this result to linear viscosity gradients, where we unveil the existence of radially constant flows and elaborate on the effect of asymmetry of the particle position within the finite-size gradient, which hitherto has not been considered.

These results are subsequently applied to bead-spring microswimmers as model systems for self-propelling active matter. In contrast to the common approach of prescribing the stroke of the swimmer, we here employ a force-based swimmer model, allowing for an adaption of the swimming stroke to the environment, and reveal the rich viscotactic properties of such a microswimmer. We also construct a simple swimmer inspired by the Chlamydomonas algae and compare the viscotactic behavior of the biological swimmer to ours.

15 min. break

CPP 22.5 Wed 10:45 H16

Noisy pursuit of active Brownian particles — •Segun Goh, Roland G. Winker, and Gerhard Gompper — IBI-5, Forschungszentrum Jülich, 52425 Jülich, Germany

Many biological and artificial agents are not only motile, but also capable of adjusting their motion based upon information gathered from their environment. This study considers sensing of a target and as a consequence reorientation of the direction of self-propulsion, which enables active pursuit. Specifically, an active Brownian particle is employed as a model agent to investigate pursuit dynamics in two dimensions, for both stationary as well as moving targets. We discuss how the interplay between intrinsic persistent self-propulsion and active reorientation by sensing gives rise to unexpected complex behaviors. In particular, the noise plays a pivotal role with both positive and negative influences on the success of pursuit. Numerical simulations and analytical calculations reveal that strong motility results in overshooting of the target, while pursuers cannot approach the target effectively at low Péclet numbers. Moreover, we propose a strategy to sort active pursuers according to their motility and reorientation capability by employing particular target trajectories.

CPP 22.6 Wed 11:00 H16

Rheotaxis of the ciliate — •Takuya Ohmura[1], Yukinori Nishigami[2], and Masatoshi Ichikawa[3] — [1]Biozentrum, University of Basel, Switzerland — [2]Research Institute for Electronic Science, Hokkaido University, Japan — [3]Department of Physics, Kyoto University, Japan

Rheotaxis, a property of organisms to move against an external flow, has a crucial role to stay in living environment. For instance, freshwater fishes in rivers swim upstream to avoid being swept away to the sea. Interestingly, recent studies reported that not only fish but also swimming cells show rheotaxis. We elucidated the rheotaxis of the ciliate, Tetrahymena, a well-known single-celled freshwater microorganism swimming by cilia [1]. While that microorganism doesn*t have a sensor to detect flow direction and micrometer-sized particles are swept away downstream in a viscous flow, what dynamics underlie the rheotaxis of the ciliate? Our experiments revealed that the ciliate slid upstream along a wall, which indicates that the cells receive rotational torque from shear flow to align swimming orientation. To evaluate the shear torque, we performed a numerical simulation with a hydrodynamic model swimmer adopting cilia dynamics in a shear flow. The result suggests that the ciliate automatically slides upstream by using cilia-stalling mechanics.

[1] T. Ohmura, et al., Science Advances, 7(43), eabi5878 (2021).

CPP 22.7 Wed 11:15 H16

Analytical study of active semiflexible ring polymer — •Christian A. Philipps, Gerhard Gompper, and Roland G. Winkler — Forschungszentrum Jülich, 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]. 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 rigidity. In contrast to linear filaments, the center-of-mass motion is independent of propulsion. However, activity strongly influences the internal dynamics with an activity enhanced diffusive for the flexible and a ballistic regime for the semiflexible ring polymer. Furthermore, a dominant rotational mode over several orders of magnitude in time emerges for high activities, which implies a rotational motion of the entire ring polymer. [1] R. G. Winkler, G. Gompper, J. Chem. Phys. 153, 040901 (2020); [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 22.8 Wed 11:30 H16

Dynamical Renormalization Group approach to the collective behavior of natural swarms — Andrea Cavagna[1], Luca Di Carlo[1], Irene Giardina[1], Tomas Grigera[1,3], •Giulia Pisegna[1,2], and Mattia Scandolo[1] — [1]Sapienza Università di Roma, Roma IT — [2]Max Planck Institute for Dynamics and Self-Organization, Goettingen DE — [3]IFLYSIB, La Plata, Argentina

Recent data on strongly correlated biological systems showed the validity of scaling laws as one of the fundamental traits of collective behaviour. Experiments on natural swarms of insects unveiled traces of critical dynamics, with inertial features and a dynamical critical exponent z=1.2. To rationalize this evidence, we develop an inertial active field theory in which the velocity is coupled to its generator of internal rotations, namely the spin, through a mode-coupling interaction. We study its near-critical regime with a one-loop Renormalization Group approach under the assumption of incompressibility. The presence of friction in the dynamics of the spin rules a paramount crossover between two fixed points: the unstable underdamped fixed point with z=1.3 and the stable overdamped fixed point with z=1.7, where dissipation takes over. We show how finite-size systems with weak dissipation, such as swarms, can actually exhibit the critical dynamics of the unstable fixed point thus providing a theoretical result which is in fair agreement with experimental data.

15 min. break

CPP 22.9 Wed 12:00 H16

Dynamics and rheology of active suspensions in viscoelastic media — •Akash Choudhary[1], Sankalp Nambiar[2], and Holger Stark[1] — [1]Institute of Theoretical Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Nordita, KTH Royal Institute of Technology and Stockholm University, Stockholm 10691, Sweden

Active suspensions are systems of motile organisms or active motors that are driven out of equilibrium through self-propulsion. This localized energy-work conversion imparts rich phenomenology and anomalous macroscale properties that are in stark contrast to passive suspensions and polymeric fluids. Motivated by the ubiquitous microbial systems in biological fluids, we analyse the impact of non-Newtonian fluids on the rheological response of active suspensions to steady shear flows.

We first study the suspension at an individual scale and show that elongated pushers (representative of *E. coli*) and pullers (*C. reinhardtii*) exhibit diverse orbital dynamics in a viscoelastic fluid. We find that the active stresses not only modify the Jeffery orbits, well-known for viscous fluids, but microswimmers can even resist flow-induced rotation and align themselves at an angle with the flow. To analyze the impact of such behavior on the bulk rheological response, we study an ensemble of a dilute suspension of such swimmers in the presence of stochastic noise from bacterial tumbling and rotary diffusion. In comparison to Newtonian media, the polymeric elastic stresses substantially and non-monotonically amplify the swimmer-induced viscosity, in particular, the superfluid transition of pusher solutions.

CPP 22.10 Wed 12:15 H16

Intercellular transport in *Chara corallina* — •Florian von Rüling[1], Anna Alova[2], Alexander Bulychev[2], and Alexey Eremin[1] — [1]Otto von Guericke University Magdeburg, Germany — [2]Moscow, Russia

We explore the kinetics of the intercellular transport between the giant cells of characean algae. The transport involves advection via cytoplasmic streaming and diffusion through the plasmodesmata, pores that penetrate the cell walls. Using fluorescent dye as a tracer, we measure the permeation through the node of tandem cells. The permeability is extracted from the experimental data using an advection-diffusion model. The current work is focused on the roles of cytoplasmic streaming and the nodal cells in the transport mechanism. To separate the diffusive permeation from the advective contribution, cyclosis was temporarily inhibited using action potentials. Streaming cessation results in dye accumulation in the vicinity of the node. The shape of regions with high dye concentration indicates that action potentials may induce closure of the plasmodesmata in central nodal cells.

CPP 23: Complex Fluids and Soft Matter 1 (joint session DY/CPP)

Time: Wednesday 9:30–12:00 Location: H18

CPP 23.1 Wed 9:30 H18

Writing in Water — •Thomas Palberg and Nadir Möller — Institut für Physik, Johannes Gutenberg Universität Mainz

Writing is an ancient cultural technique, typically performed by leaving some trace in or on a solid surface. We here explore the possibilities of leaving the trace in a liquid medium close to a surface and obtain lines or letters with high contrast and durability. Ion exchange (IEX) resin beads are used as mobile proton or hydroxyl ion sources. Moving them across the substrate in low-salt water, leaves a pH trace. Added autonomously swimming particles are able to follow this trace, mimicking hunter and prey dynamics or mate tracing, but without leaving a visible testimony. Written lines are realized by adding larger amounts of micron-sized passive particles, which settle to the like-charged substrate. Being phoretically drawn to or repelled from the pH traces, they form a well-visible trail behind the source. Trails of cationic IEX are white on black, those of anionic IEX are black on white. Their diffusive fading is slowed by continued phoretic flows and trails are stable up to hours. Sources moving autonomously just scribble. Sources propelled straight by gravity leave high-contrast lines. Deliberate tilting sequences for the substrate, then, facilitate writing.

CPP 23.2 Wed 9:45 H18

Composition Dependent Instabilities in Mixtures With Many Components — •Filipe Thewes, Matthias Krüger, and Peter Sollich — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Understanding the phase behavior of mixtures with many components is a key step towards a physics-based description of intracellular compartmentalization. We study the instabilities of a model where the interactions as quantified by the second virial coefficients are taken as random Gaussian variables. Using tools from free probability theory we obtain the spinodal curve and the nature of instabilities for an arbitrary distribution of components, thus lifting the drastic simplification of uniform composition that has been made in earlier work. We illustrate our results with examples and show that, by controlling the density of only a few components, one can systematically change the nature of instabilities and achieve demixing for realistic scenarios, which appeared to be ruled out by previous studies. Inspired by these results, we introduce an additive model taking into account also deterministic interactions. We show how this systematic interaction leads to a competition between different forms of instabilities that can be tuned by controlling the model parameters. Since most experimental protocols for complex mixtures rely on tuning either the composition or systematic interactions, we expect our results to significantly extend the range of mixtures that can be treated within the mean-field model.

CPP 23.3 Wed 10:00 H18

Phase behaviour of mixtures of hard spheres and hard rods — •Poshika Gandhi[1], Joeri Opdam[2], Anja Kuhnhold[1], Tanja Schilling[1], and Remco Tuinier[2] — [1]Institute of Physics, Albert-Ludwigs-University Freiburg, Germany — [2]Institute for Complex Molecular Systems, Eindhoven University of Technology, The Netherlands

Phase behaviours of complex mixtures are challenging to predict. A binary mixture of hard spherocylinders (HSC) and hard spheres (HS) is one such system. As rod-like particles have large excluded volume, a free volume theory (FVT) can be used to gain insights into demixing phenomenon and phase stability.

Vliegenthart *et al*[1] modified an existing FVT for binary mixtures of HS to accommodate HSC. This FVT works well for the needle limit, i.e., weak excluded volume interactions between HSC. It, however, predicts the phase boundaries at too low HSC concentrations. Opdam *et al*[2] showed that by incorporating excluded volume interactions between the depletants even in the reservoir improves the FVT significantly.

We used the new FVT to predict phase boundaries of colloidal mixtures and compared them to MC simulations. The results show that accounting for all the excluded volumes of all the components may be pivotal in understanding phase behaviour of colloidal mixtures [3].

[1] G. A. Vliegenthart et al., J. Chem. Phys., **111**, 4153 (1999).

[2] J. Opdam, et al., J. Chem. Phys., **154**, 204906 (2021)

[3] J. Opdam, et al., Phys. Chem. Chem. Phys., **24**, 11820 (2022)

CPP 23.4 Wed 10:15 H18

Markov State Modelling of Self Assembling Colloidal Systems — •Salman Fariz Navas and Sabine H.L. Klapp — ITP, Technische Universität Berlin, Germany

Many colloidal particle systems display self-assembly phenomena yielding, e.g., clusters or gel-like materials. The current project focuses on the use of phase space discretization techniques towards developing a coarse-grained description of self-assembly processes in colloidal systems.

Specifically, we develop a corresponding Markov State Model from particle-resolved Brownian Dynamics simulations, wherein the Markov states are the various local structural configurations present in the system and the Markovian process describing the stochastic transition of particles from one structure to the other.

The specific self-assembly problem studied here involves the aggregation of colloidal particles with field-induced multipolar interactions [1]. We use bond orientational order parameters and the coordination number as parameters to define the discrete states. The number of particles in the largest cluster in the system (n) is used as a parameter to quantify the progress of the overall aggregation. Transition probability matrices (TPM) between the different states are then computed for each value of n. Information regarding relaxation times and pathways relevant to the aggregation process are extracted by analyzing changes in the TPM elements.

[1] Florian Kogler, Orlin D. Velev, Carol K. Hall and Sabine H. L. Klapp, Soft Matter 11, 7356 (2015)

CPP 23.5 Wed 10:30 H18

Repulsion of topological defects in quasi-2D liquid crystal films — •Kirsten Harth[1,2] and Ralf Stannarius[3] — [1]Fachbereich Technik, TH Brandenburg, Brandenburg an der Havel, Deutschland — [2]MARS und MRTM, Otto von Guericke Universität Magdeburg, Deutschland — [3]Institut für Physik und MARS, Otto von Guericke Universität Magdeburg, Deutschland

The dynamics of topological defects is of interest, e.g., in phase transitions, cosmology or structural organization of colloids and active matter. Liquid crystals are a straightforward system allowing optical characterization of defect motion. As anisotropic fluids, they are characterized by orientational order, introducing long-range elastic forces, in addition to liquid-like fluidity with viscosity coefficients related to, e.g., the local shear flow directions respective to the local orientational field. This causes intriguing effects and must not be neglected.

The comparison of recent exeriments [1,2] in free-standing smectic C films to theoretical and numerical predictions [2,3] leaves a number of questions unanswered. A proper consideration of flow coupling and / or of an anistropy of the elastic constants in a simulation with realistic boundary conditions may solve the issues. We explain why elastic anisotropy is particularly important here. Experimental and numerical data are compared to elucidate the effect of elastic constants and flow on the repeulsion dynamics.

[1] A. Missaoui, et al., PR Research 2 013080 (2020). [2] R. Stannarius, K. Harth, PRL 117 157801 (2016). [3] e.g. X. Tang, J. V. Selinger, Soft Matter 13 5481 (2017) ; Soft Matter, 15 587 (2019)

15 min. break

CPP 23.6 Wed 11:00 H18

Incipient motion for 3d geometries — •Dominik Geyer, Paolo Malgaretti, Othmane Aouane, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (IEK-11), Cauerstr. 1, 91058 Erlangen, Germany

The incipient motion describes the threshold conditions between erosion and sedimentation. This natural process is relevant for a broad field of natural and industrial processes, for example, cell detachment, cleaning of surfaces, and transportation in pipelines. Our interest is in the incipient motion of a single particle on non-trivial geometries. The crucial parameter for describing incipient motion is the so-called Shields number which is the ratio between viscous forces and buoyancy. Interestingly, the incipient motion has been reported at values of the Shields number much smaller than unity ($\theta \simeq 10^{-2}$) hence questioning whether the proposed Shields number is indeed capturing the relevant physical phenomena. In order to critically discuss this aspect, we perform lattice Boltzmann simulations of a solid particle on a substrate consisting of solid spheres taking into account the local fluid velocity and the particle size. Our numerical data will allow us to calculate the effective viscous force acting on the particle and hence to propose possible corrections to the Shields number which can better account for the experimental and numerical data.

CPP 23.7 Wed 11:15 H18

Phase behaviour in a mono-layer colloidal membrane — •Léa Beaules, Anja Kuhnhold, and Tanja Schilling — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

Kosterlitz-Thouless-Halperin-Nelson and Young (KTHNY) theory predicted that the melting of a purely 2D hard disk system would be defect-mediated and occur via two continuous transitions: from the solid to the intermediate hexatic phase and, from the hexatic to the fluid phase. Since then phase behaviour of this system as well as closely related systems have been extensively investigated and debated, showing that the hexatic-liquid transition is of first order for purely hard system [1]. Additionally, upon increasing interaction range or adding dispersity in the system the transition can become continuous or the hexatic phase can vanish [2].

However a large number of real systems can be more accurately approximated as a quasi-2D system that exhibits out of plane interactions, e.g. biological membranes; therefore understanding their role in the phase behaviour is important. Thus to extend our understanding of these systems, we use Monte-Carlo simulations to study an infinite mono-layer membrane of hard rod-like particles. We investigate how the orientational degree of freedom of the rods, and the range of their out of plane interactions affect the phase behaviour of the system.

[1] E. P. Bernard and W. Krauth, Phys. Rev. Lett. **107**, p. 155704 (2011).

[2] Y.-W. Li and M. P. Ciamarra, Phys. Rev. E **102**, p. 062101 (2020).

CPP 23.8 Wed 11:30 H18

Particle-resolved topological defects of smectic colloidal liquid crystals in 2d confinement — •René Wittmann[1], Paul A. Monderkamp[1], Louis B. G. Cortes[2,3], Dirk G. A. L. Aarts[3], Frank Smallenburg[4], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Germany — [2]School of Applied and Engineering Physics, Cornell University, USA — [3]Department of Chemistry, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK — [4]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, France

We present a general classification scheme [1] of the intrinsic structure of smectic colloidal liquid crystals in two spatial dimensions, dictated by the interplay between the intrinsic layering and the externally imposed boundary structure. Thereby, we demonstrate that topological defects emerge in the form of spatially extended grain-boundaries, which are characterized by coexisting nematic and tetratic orientational order. We examine these intriguing topological properties on the particle scale by means of Monte-Carlo simulations, fundamental-measure-based density functional theory and real-space microscopy of colloidal rods. The structural details agree on a quantitative level. In particular, we analyze the typical shape of grain-boundary networks in a large range of polygonal confinements [1] and the stability of different competing topological states in nontrivial domains with additional interior boundaries [2].

[1] P. A. Monderkamp et al., Phys. Rev. Lett. 127, 198001 (2021).

[2] R. Wittmann et al., Nat. Commun. 12, 623 (2021).

CPP 23.9 Wed 11:45 H18

Structure of nematic hard rod tactoids — •Anja Kuhnhold[1] and Paul van der Schoot[2] — [1]University of Freiburg, Freiburg, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands

Droplets of ordered phases of anisotropic particles take on specific shapes and internal structures. Compared to droplets of spherical particles, tactoids are elongated with cusp-like tips. Several parameters dictate the overall shape and structure: density of the system, elastic constants of the particles, anchoring strength, interfacial tension, and volume of the tactoid. [1]

We compare Monte Carlo simulation results of hard rod tactoids in a bath of spherical ghost particles to predictions from a scaling theory. We focus on small tactoids where the macroscopic scaling description might break down. We find that smaller tactoids have a more uniform director field than larger tactoids. Also, the segment density increases towards the tactoid tips in agreement with the theory. In addition, we find further density modulations when the average density increases.

Besides, we test the effect of an aligning field on the shape and structure of the tactoids and find that the director field becomes more uniform and the aspect ratio increases, but not to a vast extent. [2]

[1] P. Prinsen, P. van der Schoot, EPJ E **13**, 35 (2004).

[2] A. Kuhnhold, P. van der Schoot, JCP **156**, 104501 (2022).

CPP 24: 2D Materials 5 (joint session HL/CPP/DS)

Time: Wednesday 9:30–12:00 Location: H36

CPP 24.1 Wed 9:30 H36

Dark exciton anti-funneling in monolayer transition metal dichalcogenides — •Roberto Rosati[1], Robert Schmidt[2], Samuel Brem[1], Raül Perea-Causín[3], Iris Niehues[4], Johannes Kern[2], Johann Adrian Preuss[2], Robert Schneider[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Ermin Malic[1,3] — [1]Philipps-Universität Marburg — [2]University of Münster — [3]Chalmers University of Technology — [4]CIC nanoGUNE BRTA

Current nanoelectronics relies on transport. While charged carriers can be controlled by electric fields, atomically thin semiconductors are governed by excitons, which are neutral electron-hole pairs. Recently, strain engineering has been introduced to manipulate exciton diffusion [1] and propagation [2] in monolayer transition metal dichalcogenides. Strain-induced energy gradients give rise to exciton funneling up to a micrometer range. Combining spatiotemporal photoluminescence measurements with microscopic theory, here we track the way of excitons in time, space and energy. Surprisingly we find that in WS_2 excitons move away from high-strain regions, contrary to what we observe in $MoSe_2$ [2]. This anti-funneling behavior can be ascribed to dark excitons, whose strain-induced energy variations are opposite compared to bright excitons. Our findings open new possibilities to control transport in exciton-dominated materials.

[1] R. Rosati et al., 2D Mater. 8, 015030 (2021).

[2] R. Rosati, R. Schmidt et al., Nat. Commun. 12, 7221 (2021).

CPP 24.2 Wed 9:45 H36

Ultrafast nanoscopy of a Mott transition in twisted bilayer WSe_2 — •Svenja Nerreter[1], Thomas Siday[1], Fabian Sandner[1], Samuel Brem[2,3], Martin Zizlsperger[1], Felix Schiegl[1], Raul Perea-Causin[3], Markus Plankl[1], Philipp Merkl[1], Fabian Mooshammer[1,4], Markus A. Huber[1], Ermin Malic[2,3], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, 93040 Regensburg — [2]Department of Physics, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Physics, Chalmers University of Technology, 41296 Gothenburg, Sweden — [4]Department of Physics, Columbia University, New York, NY 10027, USA

The density-driven transition of an exciton gas into a Fermi liquid of unbound electron-hole pairs has formed a compelling testing ground of many-body physics. Layered transition metal dichalcogenides feature advantageous conditions, yet nanoscale inhomogeneities have complicated quantitative studies of this elusive transition. Here, we use ultrafast polarization nanoscopy to trace optically bright and dark electron-hole pairs during an exciton Mott transition in a twisted homobilayer of WSe_2. At elevated densities, initially monomolecular recombination dynamics of optically dark excitons continuously evolve into the bimolecular recombination of unbound electron-hole pairs. We directly reveal how the Mott transition varies over nanometer length scales, evidencing strong spatial disorder in stacked monolayers and demonstrating the capabilities of our technique to resolve the local interplay of strong electronic correlations.

CPP 24.3 Wed 10:00 H36

Rashba excitons in the 2D Ruddlesden-Popper perovskite (BA)MAPI — •Philipp Moser[1], Martin Schalk[1], Atsuhiko Miyata[2], Joachim Wosnitza[2], Andreas Stier[1], and Jonathan Finley[1] — [1]Walter Schottky Institute, Garching, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Two-dimensional organic-inorganic perovskites have emerged as remarkable materials for energy conversion, optoelectronic and spintronic applications. Recently, the role of spin-orbit (SO) coupling and the resulting effects on the band-structure and dark/bright optical transitions has become a key topic of interest. The necessary structural inversion asymmetry for SO-coupling is predicted to stem from the organic cations comprising the crystals. As a result, dark excitons, red detuned from the bright exciton, have been discussed in this material system. Here, we investigate the exciton physics of the 2D Ruddlesden-Popper perovskite (BA)MAPI. By performing one-photon absorption, -PL and two-photon PLE spectroscopy, we investigate the optical transitions close to the R-point of the Brillouin zone and find distinct 2-photon transitions blue detuned from the ground state exciton that can be explained by a Rashba-split band-structure. Utilizing high-field magneto-spectroscopy up to B=60T, we determine that these absorption features are due to Wannier excitons. We determine the size and binding energy from the diamagnetic shift of the features and obtain evidence that 2D (BA)MAPI hosts strongly bound Rashba excitons.

CPP 24.4 Wed 10:15 H36

Ultrafast pseudospin quantum beats in multilayer WSe2 and MoSe2 — •Simon Raiber[1], Paulo E. Faria Junior[2], Dennis Falter[1], Simon Feldl[1], Petter Marzena[1], Kenji Watanabe[3], Takashi Taniguchi[4], Jaroslav Fabian[2], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

We present investigations of excitonic transitions in mono- and multilayer WSe2 and MoSe2 materials by time-resolved Faraday ellipticity (TRFE) with in-plane magnetic fields, of up to B = 9 T. In monolayer samples, the measured TRFE time traces are almost independent of B, which confirms a close to zero in-plane exciton g factor, consistent with first-principles calculations. In stark contrast, we observe pronounced temporal oscillations in multilayer samples for $B > 0$. Remarkably, the extracted in-plane g factors are very close to reported out-of-plane exciton g factors of the materials, namely $|g< 1s| = 3.1$ +/- 0.2 and 2.5 +/- 0.2 for the 1s A excitons in WSe2 and MoSe2 multilayers, respectively. Our first-principles calculations nicely confirm the presence of a non-zero in-plane g for the multilayer samples. We propose that the oscillatory TRFE signal in the multilayer samples is caused by pseudospin quantum beats of excitons, which is a manifestation of spin- and pseudospin layer locking in the multilayer samples.

CPP 24.5 Wed 10:30 H36

Nonlinear Exciton Dynamics in Layered Heterostructures — •Vipin Krishna[1], Xiao Chen[2], Tarlan Hamzayev[1], Silvana Botti[2], and Giancarlo Soavi[1] — [1]Institute of Solid state Physics,Friedrich-Schiller-University,Jena — [2]Institute of Theoretical Solid State Theory and Optics,Friedrich-Schiller-University,Jena

Transition-metal-dichalcogenides and related heterostructures(HS) are promising candidates for photonic and optoelectronic applications owing to strong light-matter coupling and electrically-tunable carrier dynamics.However,the presence of intense nonlinear effects such as Exciton-Exciton Annihilation(EEA)[1] limits the maximum realizable exciton-density,and is particularly efficient for interlayer-excitons(IL) due to their out-of-plane dipole nature[2].In this work,we systematically study the onset of EEA in type-II WS2/WSe2 HS by steady-state and nonlinear time-resolved PL.We infer that in HS the generation-rate is at least one order of magnitude larger for interlayer compared to intralayer-excitons for a given excitation-fluence, as expected from the ultrafast interlayer-charge-transfer and consequent IL formation.However,we do not observe stronger EEA for interlayer compared to intralayer-excitons and observe that for HS the recombination-dynamics are identical for both,suggesting that the EEA mechanism is dominated by the total excitonic-density via intra and interlayer-exciton interactions.Our work provides new insights on EEA mechanism, which is of paramount importance for optoelectronic-devices and study of excitonic-condensates with layered-materials.[1]Kuechle et.Al.J.OMX(2021),12.[2]Sigl et.Al.Phys.Rev.B 105,035417.

15 min. break

CPP 24.6 Wed 11:00 H36

Tunable exciton-polaritons emerging from WS_2 monolayer excitons in a photonic lattice at room temperature — •Lukas Lackner[1], Marco Dusel[2], Oleg Egorov[3], Bo Han[1], Heiko Knopf[3], Falk Eilenberger[3], Carlos Anton-Solanas[1], Sven Höfling[2], and Christian Schneider[1] — [1]University of Oldenburg, Oldenburg, Germany — [2]University of Würzburg, Würzburg, Germany — [3]Friedrich Schiller University Jena, Jena, Germany

The engineering of non-linear light-matter states in optical lattices has emerged as a key research strategy for the exploration of Hamiltonians in the spirit of ultrafast- and possibly quantum-simulation. It furthermore has revealed its potential to probe non-trivial topology phenomena. Excitons in atomically thin crystals have emerged as an ideal active medium for such purposes, since they couple strongly with light, and bear the potential to harness giant non-linearities and interactions.

In this work, we present an experiment conducted at room temperature in an open optical cavity of high quality, with an implemented one-dimensional photonic lattice. In our present work we integrate an atomically thin layer of WS_2 in such a device. We discuss the emergence and tunability of a lattice-band-structure in the tight-binding configuration at room temperature, fuelled by the emission from monolayer excitons[1].

References

[1] L. Lackner *et al., Nat Commun* **12**, 4933 (2021).

CPP 24.7 Wed 11:15 H36

Optical Spectroscopy of Colloidal Transition Metal Dichalcogenides — •André Philipp Frauendorf[1], André Niebur[2], Jens Hübner[1], Jannika Lauth[2,3], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover — [3]Institut für Physikalische und Theoretische Chemie, Universität Tübingen

Atomically thin transition metal dichalcogenides (TMDs) are at the forefront of a new generation of two-dimensional semiconductor systems and experience an increasing research interest due to their unique optical properties. As an additional fabrication approach the wet-chemical synthesis has emerged as a promising method for the straightforward solution-processing of these materials. [1] Nevertheless, the optical properties of colloidal TMD mono- and few-layer structures have been sparsely studied.

Here, we demonstrate room-temperature micro-photoluminescence of colloidal TMD nanosheets. Both, mono-and multilayer photoluminescence are observed rendering these delicate structures fully competitive with conventionally fabricated TMDs. [1] In addition temperature-dependent transient absorption measurements are presented as a convincing technique for the exploration of the ultra-fast recombination dynamics of two-dimensional materials. [2]

[1] A. Frauendorf et al., J. Phys. Chem. C 125, 18841 (2021).

[2] A. Frauendorf et al., Manuscript in preparation (2022).

CPP 24.8 Wed 11:30 H36

Capacitively and inductively coupled excitons in bilayer MoS_2 — •Lukas Sponfeldner[1], Nadine Leisgang[1], Shivangi Shree[2], Ioannis Paradisanos[2], Kenji Watanabe[3], Takashi Taniguchi[4], Cedric Robert[2], Delphine Lagarde[2], Andrea Balocchi[2], Xavier Marie[2], Iann C. Gerber[2], Bernhard Urbaszek[2], and Richard J. Warburton[1] — [1]Department of Physics, University of Basel — [2]Université de Toulouse, INSA-CNRS-UPS, LPCNO — [3]Research Center for Functional Materials, National Institute for Materials Science — [4]International Center for Materials Nanoarchitectonics, National Institute for Materials Science

Exciton-exciton couplings in semiconductors lead to a plethora of phenomena such as nonlinear optical effects and quantum condensation. Transition-metal dichalcogenides constitute a versatile platform to study these effects as the excitons are very robust and their couplings can be controlled by exploiting their spin and valley properties.

Here, we probe exciton-exciton couplings in gated-homobilayer MoS_2. Using a driven-coupled oscillator model it is shown that the measured optical susceptibility reveals both the magnitude and the phase of the coupling constants. The interlayer excitons (IE) and intralayer B-excitons couple via a 0-phase (capacitive) coupling; the IE and the intralayer A-excitons couple via a π-phase (inductive) coupling. Using the IE as a sensor, the A-B intravalley exchange coupling is determined, a result which is also relevant for a monolayer. Finally, we realize a bright and highly tunable lowest-energy momentum-direct exciton at high electric fields.

CPP 24.9 Wed 11:45 H36

Controlling the non-linearity in two dimensional materials — •Mathias Federolf and Sven Höfling — Technische Physik, Universität Würzburg, 97074 Würzburg, Germany

Recently Datta et al. [1] have shown that exciton-polaritons in bilayer MoS_2 experience a blueshift due to interacting with other exciton-polaritons. The observed blueshift is non-linear with respect to the laser power used for excitation. Due to the bilayer's nature interlayer-excitons can occur, which exhibit an out of plane dipole moment. Using an electric field along the out of plane axis those dipoles can be aligned and used to influence the exciton-exciton interaction. By using a varying electric field, we map the parameter space to gain deterministic control over the blueshift. Understanding and controlling the system allows us to tune the polariton-polariton interaction such that they can be used in future application i.e., single-photon sources.

[1] Datta, Biswajit, et al. arXiv preprint arXiv:2110.13326 (2021).

CPP 25: 2D Materials 6 (joint session DS/CPP)

Time: Wednesday 11:15–13:00 Location: H17

CPP 25.1 Wed 11:15 H17

Curvature-induced spin-orbit splitting in transition metal dichalcogenide nanotubes and wrinkles — Mohammadreza Daqiqshirazi and •Thomas Brumme — Theoretical Chemistry, TU Dresden

Strain engineering provides a powerful means to tune the properties of 2D materials. Homogeneous strain fields have been studied extensively, and there are standard techniques for altering properties of 2D materials even in industry. On the other hand, much less is known about how inhomogeneous strain affects the electronic properties of 2D materials. We employed DFT to understand the correlation between the atomic and the electronic structure in nanoscale wrinkles and nanotubes of the prototypical transition metal dichalcogenide WSe_2. Our research shows that the symmetry breaking in these structures lead to strong Rashba-like spin-orbit splitting of the bands at the Γ point and that they thus may be utilized in future tunable spintronics devices.

CPP 25.2 Wed 11:30 H17

Moiré-Bose-Hubbard model for interlayer excitons in twisted transition metal dichalcogenide heterostructures — •Niclas Götting, Frederik Lohof, and Christopher Gies — Institute for Theoretical Physics, University of Bremen, Bremen

Introducing a twist between two superimposed TMD monolayers results in a new superlattice whose properties heavily depend on the twist angle. These so-called moiré structures of TMD materials like MoS_2/WS_2 can host interlayer excitons (IXs) which perceive the varying atomic registry over the moiré unit cell as an effective moiré potential. In such structures, correlated states can emerge, in which the IXs are strongly localized to the potential minima due to exciton-exciton interactions.

We investigate the phases of these trapped moiré IXs by approximating them as bosonic particles and mapping the system onto a Bose-Hubbard model [1]. Our methods allow us to calculate the hopping and two-particle interaction terms of the Bose-Hubbard model for n-th nearest neighbors. To examine the strong impact of dielectrics surrounding the heterobilayer, we introduce a Keldysh potential to the calculation and thereby obtain first results of the twist-angle dependent phases of moiré IXs in twisted TMD heterobilayers.

[1] Götting et al., Phys. Rev. B 105, 165419 (2022)

CPP 25.3 Wed 11:45 H17

Enhanced Potassium Storage Capability of Two-Dimensional Transition-Metal Chalcogenides — •Vincent Hartmann and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Potassium-ion batteries (PIBs) have been considered a promising alternative to lithium-ion batteries due to their merits of high safety and low cost. Two-dimensional transition metal chalcogenides (2D TMCs) with high theoretical specific capacities and unique layered structures have been proven to be amenable materials for PIB anodes. However, some intrinsic properties including severe stacking and unsatisfactory conductivity restrict their electrochemical performance, especially rate capability. Herein, a heterostructure of high-crystallized ultrathin MoSe2 nanosheet-coated multiwall carbon nanotubes was prepared and its electrochemical properties were investigated. In such a heterostructure, the constructive contribution of CNTs not only suppresses the restacking of MoSe2 nanosheets but also accelerates electron transport. Meanwhile, the MoSe2 nanosheets loaded on CNTs exhibit an ultrathin feature, which can expose abundant active sites for the electrochemical reaction and shorten the K+ diffusion length. Therefore, the synergistic effect between ultrathin MoSe2 and CNTs endows the resulting nanocomposite with superior structural and electrochemical properties. Additionally, the high crystallinity of the MoSe2 nanosheets further leads to the improvement of electrochemical performance.

CPP 25.4 Wed 12:00 H17

Single photon emission of quantum emitters in WSe2 monolayers and their temperature-dependent coherence properties — •Martin von Helversen[1], Paul Schlaugat[1], Chirag Palekar[1], Carlos Antón-Solanas[2], Bárbara Rosa[1], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institute for solid state physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Institute for Physics, Carl von Ossietzky Universtität Oldenburg, 26111 Oldenburg, Germany

Two-dimensional van der Waals monolayers have appeared as novel type of semiconducting materials, which provide a platform for the exploration of their highly interesting optical, electronic and structural properties. Within the transition-metal dichalcogenides, WSe2 has turned out to be the most promising platform for two-level single-photon emitters, generated either by applied strain to the monolayer-flake [1,2], or by defects in the material [2]. However, the quality of the generated photons still lacks behind other systems as for example semiconductor quantum dots. In this work, we study single emitters of a strained WSe2-monolayer showing linewidths around 100 μeV at 4 K. In quasi-resonant pulsed optical excitation a second-order autocorrelation value down to $g^{(2)}(0)=0.037(5)$ is measured. We further study their temperature dependent first-order coherence properties via a scanning Michelson interferometer, which yields coherence times up to 48 ps.
[1] L. N. Tripathi et al., ACS Photonics 5, 1919 (2018)
[2] K. Parto et al., Nat. Commun. 12, 3585 (2021)

CPP 25.5 Wed 12:15 H17

Spin-defect characteristics of single sulfur vacancies in monolayer MoS$_2$ — •Alexander Hötger[1], Tomer Amit[2], Julian Klein[3], Katja Barthelmi[1], Thomas Pelini[4], Alex Delhomme[4], Sergio Rey[5], Marek Potemski[4,6], Clément Faugeras[4], Galit Cohen[2], Daniel Hernangómez-Pérez[2], Takashi Taniguchi[7], Kenji Watanabe[7], Christoph Kastl[1], Jonathan Finley[1], Sivan Refaely-Abramson[2], Alexander Holleitner[1], and Andreas Stier[1] — [1]Walter Schottky Institute, Garching, Germany — [2]Weizmann Institute of Science, Rehovot, Israel — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Laboratoire National des Champs Magnetiques Intenses, Grenoble, France — [5]Technical University of Denmark, Lyngby, Denmark — [6]University of Warsaw, Warszawa, Poland — [7]National Institute for Materials Science, Tsukuba, Japan

Single spin defects in 2D transition-metal dichalcogenides are natural spin-photon interfaces for quantum applications. Here we report high-field magneto-spectroscopy from three emission lines of He-ion induced sulfur vacancies in monolayer MoS$_2$. The distinct valley-Zeeman splitting and the brightening of dark states necessitates spin-valley selectivity of the defect states and lifted spin-degeneracy at zero field. Comparing our results to ab-initio calculations identifies the nature of the defect luminescence. Analysis of the optical degree of circular polarization reveals that the Fermi level is a parameter that enables the tunability of the emitter. These results show that defects in 2D semiconductors may be utilized for quantum technologies.

CPP 25.6 Wed 12:30 H17

Probing excitonic population dynamics by nonlinear optical wave mixing in monolayer WSe2 — •Jonas M. Bauer, Lijue Chen, Philipp Wilhelm, Sebastian Bange, John M. Lupton, and Kai-Qiang Lin — Department of Physics, University of Regensburg, 93053 Regensburg, Germany

Monolayer semiconductors are emerging platforms for strong nonlinear light-matter interaction, due to their giant oscillator strength of tightly bound excitons. Recently, we reported the existence of a new excitonic species, the high-lying exciton (HX), in monolayer WSe2. The HX appears at around twice the energy of the band-edge A-exciton, forming a ladder-type excitonic three-level system. We demonstrate excitonic quantum interference in monolayers [1] and twisted bilayers [2]. Here, we apply time-resolved nonlinear spectroscopy to probe the excitonic dynamics. We find that a significant time difference between two light pulses is necessary for optimal sum-frequency generation (SFG) and four-wave mixing (FWM) if one of the pulses is in resonance with an excitonic transition. The experimental results are rationalized by numerical calculations based on a density-matrix approach and provide insights into coherent exciton dynamics on a femtosecond scale.

[1] K.-Q. Lin, S. Bange, & J. M. Lupton, Nat. Phys. 15, 242-246 (2019).

[2] K.-Q. Lin, J.M. Bauer et al., Nat. Commun. 12, 1553 (2021).

CPP 25.7 Wed 12:45 H17

Characterization of 2D WSe2 by high-resolution STEM and Differential Phase Contrast STEM — •Maja Groll[1], Julius Bürger[1], Ioannis Caltzidis[2], Marc Sartison[2], Klaus Jöns[2], and Jörg Lindner[1] — [1]Nanostructuring, Nanoanalysis and Photonic Materials Group, Department of Physics, Paderborn University, Germany — [2]Hybrid Quantum Photonic Devices, Department of Physics, Paderborn University, Germany

2D transition metal dichalcogenides (TMDs) are gaining attention as their optical and electronic properties differ from those of their bulk counterparts. In particular, layer thickness-dependent properties, such as the transition from an indirect to a direct band gap in monolayers, make these materials interesting for photonic and optoelectronic applications. At the same time 2D-TMDs are ideal materials for the advancement of new techniques in scanning transmission electron microscopy (STEM) like differential phase contrast (DPC)-STEM. Using a spherical aberration corrected STEM, this technique enables the quantification of atomic electric fields with sub-atomic resolution if the specimen is sufficiently thin. In order to examine the atomic electric fields of TMDs, we transferred mechanically exfoliated mono- and multilayers of tungsten diselenide (WSe2) to TEM grids. The atomic structure of WSe2 flakes and their thickness are studied using TEM, energy filtered TEM and STEM. STEM-DPC measurements are performed using an eight-fold segmented bright-field STEM detector measuring the beam deflection due to the internal fields. Results are presented for WSe2 flakes of different thickness and compared with simulations.

CPP 26: Organic Electronics and Photovoltaics 2

Time: Wednesday 11:30–13:00 Location: H38

CPP 26.1 Wed 11:30 H38

Large Area Semitransparent Near-Infrared Organic Photodetectors — Yazhong Wang[1], •Tianyi Zhang[1], Louis Conrad Winkler[1], Donato Spoltore[2], Johannes Benduhn[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [2]Department of Mathematical, Physical and Computer Sciences, University of Parma, V.le delle Scienze 7/A, 43124 Parma, Italy

Organic photodetector (OPD) is a promising technology for several sensing applications. With advances in material synthesis and device engineering, OPDs can rival their inorganic counterparts due to their tunable absorption, lightweight, facile fabrication, low cost, and comparable performance. Here, we demonstrate a semi-transparent large area (256 mm^2) near-infrared OPD. Through vacuum deposition and optimization of the thickness of the back metal contact layer, a promising average visible transmittance up to 34.6% is achieved while maintaining 36.0% of external quantum efficiency at 790 nm. Judicious design for combining wide-optical gap buffer layers with semitransparent electrodes results in the remarkable specific detectivity of 1.4×10^{13}(6.44 mm^2) and 1.1×10^{12}(large area) Jones, respectively. Those performances are comparable with commercial silicon photodiodes. To the best of our knowledge, our device is the best see-through, large-area, near-infrared OPD, which enables a higher level of photon detection and integration into image sensors. The transparency and good stability of these OPDs make them excellent candidates for various biomedical sensing applications and the internet of things.

CPP 26.2 Wed 11:45 H38

Exploring Highly Ordered Rubrene:C_{60} Heterojunctions for Organic Photodetectors — •Anna-Lena Hofmann[1], Lucy Winkler[1], Max Herzog[1], Eva Bittrich[2], Jakob Wolansky[1], Martin Kroll[1], Johannes Benduhn[1], and Karl Leo[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany — [2]Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Rubrene can form highly ordered phases, demonstrating an unusually high charge carrier mobility for holes ($> 10\,\mathrm{cm^2V^{-1}s^{-1}}$) even in thin films. Therefore it is a promising material for high-performance organic photodetectors (OPDs). To study the impact on OPDs, crystalline triclinic rubrene is compared to amorphous rubrene. Planar heterojunctions (PHJs) and bulk heterojunctions (BHJs) are fabricated for both material systems. For the latter, rubrene is doped with 2, 5, and 10 wt% of C_{60}. Linearly polarized microscopy is used to get the first insight into the morphology, which is then completed by ellipsometry, atomic force microscopy (AFM), and x-ray diffraction (XRD). For the electrical characterization, the external quantum efficiency (EQE) and IV characteristics are obtained, where an additional crystalline sample with a neat C_{60} layer is investigated. The neat layer of C_{60} achieves an enormous improvement of the EQE. This makes the PHJ a more favourable device architecture. Even though triclinic rubrene reaches a higher EQE and has a broader spectral response, it does underperform in optimized OPDs concerning the specific detectivity since the dark current is three magnitudes higher than the amorphous counterpart.

CPP 26.3 Wed 12:00 H38

Hybrid Energy Harvester based on Triboelectric Nanogenerator and PbS Quantum Dot Solar Cell — •Tianxiao Xiao[1], Wei Chen[1], Wei Cao[1], and Peter Müller-Buschbaum[1,2] — [1]Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

Developing clean energy lies in the heart of the sustainable development of human society. Triboelectric nanogenerators (TENGs) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to the light-weight, low-cost, and easy fabrication TENGs become one of the most promising candidates in the replacement of conventional fossil fuels and attract 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 dot (QD) based solar cell component, which can harness both mechanical and solar energy from ambient environment to directly generate electricity.

CPP 26.4 Wed 12:15 H38

***In Situ* and *In Operando* KPFM Studies on OFET Based on Hexadecafluoro-Copper-Phthalocyanine ($F_{16}PcCu$) to Access Energy Level Alignment and Electrical Contact Resistance** — •Pascal Schweitzer, Clemens Geis, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Contact resistances are considered a show-stopper for organic field effect transistors (OFET). Perfluorinated copper-phthalocyanine ($F_{16}PcCu$) is a promising chemically stable n-conductor to build complementary logical circuits with established p-conductors. A reasonably high charge carrier mobility $\mu_{ext} \approx 2 \times 10^{-3}\mathrm{cm^2/Vs}$ was estimated from device performance affected, however, by neglected contact resistances. In this work, we used *in operando* Kelvin probe force microscopy under high vacuum to study the influence of contact resistances at the source and drain electrodes on the OFET performance. Non-contact potentiometry at different applied external voltages revealed relevant voltage drops at the electrode interface and in the adjacent contact region. Based on these voltage drops and measured device currents significant contact resistances were calculated. Correcting for such parasitic voltage drops, contact-free μ_{ch} was obtained, substantially higher than μ_{ext}. The growth mode of $F_{16}PcCu$ on application-relevant polycrystalline gold substrates and shifts of the energy levels were studied by *in situ* KPFM and an injection barrier was confirmed. From these results, we conclude that the model of thermionic emission, often used for contact resistances, is not completely sufficient to describe the present case.

CPP 26.5 Wed 12:30 H38

Thin films of electron donor-acceptor complexes: characterisation of mixed-crystalline phases and implications for electrical doping — •Andreas Opitz[1], Giuliano Duva[2], Marius Gebhardt[3], Hongwon Kim[3], Eduard Meister[3], Tino Meisel[1], Paul Beyer[1], Valentina Belova[2], Christian Kasper[4], Jens Pflaum[4], Linus Pithan[4,5], Alexander Hinderhofer[2], Frank Schreiber[2], and Wolfgang Brütting[3] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Germany — [3]Institut für Physik, Universität Augsburg, Germany — [4]Experimentelle Physik VI, Julius-Maximilians-Universität Würzburg, Germany — [5]European Synchrotron Radiation Facility, Grenoble Cedex 9, France

Electron donor-acceptor (EDA) complexes are of interest as low-band gap molecular semiconductors and as dopants for molecular semiconducting matrices. Our recent work establishes a link between optical, structural and vibrational properties of EDA complexes as well as the electrical doping by them. [1] Here, we report on optical and electrical properties of EDA complexes. All studied donor:acceptor systems form mixed crystalline structures and the EDA complex is characterised by the complex-related absorption, which cross the neutral-to-ionic boundary. Our measurements reveal an exponential relation between electrical conductivity and activation energy of transport for all complex-doped systems related to the separation of Coulombically bound charges.

[1] A. Opitz *et al.*, *Mater. Adv.* **3** (2022). DOI: 10.1039/D1MA00578B

CPP 26.6 Wed 12:45 H38

Effect of phenylation vs. functionalization for tetracene-based electron transport materials — •Maryke Kouyate, Sebastian Hutsch, and Frank Ortmann — Technical University of Munich, Munich, Germany

In analogy to the tetracene/rubrene system, new electron transport materials (ETMs) are designed by modifying the outer benzene rings of tetracene with electron-withdrawing groups and attaching four phenyl groups to the modified backbone. Subsequent crystal structure prediction and charge transport calculations provided further insights in the structural effect of tetra-phenylation on tetracene based systems and the impact on charge transport properties. A strong effect of core-end modification on the molecular packing and charge transport properties for molecules without phenylation is revealed. These structures differ significantly from the known crystal structure of tetracene. Tetraphenylation, on the other hand, reduces the impact of core-end modification and crystal structures close to the high-mobility orthorhombic rubrene structure are obtained, suggesting a considerable steric effect of the bulky phenyl-groups. We finally compare the charge-transport properties between the tetracene/rubrene reference systems and ETMs with and without phenyl functionalization.

CPP 27: Composites and Functional Polymer Hybrids

Time: Wednesday 11:30–13:00 Location: H39

CPP 27.1 Wed 11:30 H39

Polymer - Organic Metal Composites for Waste Heat Recovery — •Marie Siegert[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The interest in organic thermoelectrics has greatly gained traction over the last decade due to its great potential in waste heat recovery based on sustainable, low-cost materials. For instance, polymers can be solution processed on industrial scale and display aptly low thermal conductivity, but lack high electrical conductivity due to their inherent disorder. Organic molecular metals, on the other hand, exhibit superior electrical conductivity over a wide temperature range, but the complexity of preparation currently limits scalable applications [1]. Here, we report on an approach utilizing suitable polymers in combination with the p-type organic metal TTT_2I_3 and the n-type $Cu(DCNQI)_2$, thus exploiting the benefits of both material classes. As demonstrated by our preliminary experimental data, these composite materials do not only allow for a controlled variation of the thermoelectric properties via the respective amount of organic metal additive but also show significant improvements with respect to their mechanical integrity upon thermal treatment. The related thermoelectric properties of the composites will be evaluated with regard to their application in thin film based organic thermolectric generators for waste heat recovery. The Deutsche Bundesstiftung Umwelt (DBU) is acknowledged for financial support.
[1] F. Huewe, A. Steeger, et al. Adv. Mat. 29 (2017) 1605682

CPP 27.2 Wed 11:45 H39

From spinning to spraying functional materials: structural and thermoelectric properties of gold doped spin-casted and spray-deposited P3HT-based thin films — •Benedikt Sochor[1], Anna-Lena Oechsle[2], Constantin Harder[1,2], Alexei Vorobiev[3,4], Peter Müller-Buschbaum[2,5], and Stephan V. Roth[1,6] — [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]Uppsala University, Department of Physics and Astronomy, Lägerhyddsvägen 1, 752 37 Uppsala, Sweden — [5]Research Neutron Source Heinz Maier-Leibnitz, FRM II, Lichtenbergstr. 1, 85748 Garching, Germany — [6]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. Upon addition of a suitable metal dopant, e.g. chloroauric acid (HAuCl4), thin P3HT films exhibit thermoelectric properties with large values for the power factor and figure of merit. To investigate the possibility and efficiency of future scalable industrial manufacturing, spin-casted and spray-deposited P3HT films were compared correlating their structural differences with their thermoelectric performance upon doping using AFM, GISAXS/GIWAXS, XRR and NR measurements.

CPP 27.3 Wed 12:00 H39

In-situ GISAXS Observation and Large Area Homogeneity Study of Slot-Die Printed PS-b-P4VP and PS-b-P4VP/FeCl3 Thin Films — •Shanshan Yin[1], Ting Tian[1], Christian L. Weindl[1], Kerstin S. Wienhold[1], Qing Ji[2], Yajun Cheng[2], Yanan Li[3], Christine M. Papadakis[3], Matthias Schwartzkopf[4], Stephan V. Roth[4,5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]NIMTE, Chinese Academy of Sciences, 315201, P. R. China — [3]TU München, Physik-Department, Fachgebiet Physik weicher Materie, 85748 Garching — [4]DESY, 22607 Hamburg — [5]Royal Institute of Technology KTH, 100 44 Stockholm — [6]MLZ, TU München, 85748 Garching

Mesoporous hematite (Fe2O3) thin films with high surface-to-volume ratios show great potential as photoelectrodes or electrochemical electrodes in energy conversion and storage. In the present work, with the assistance of an up-scalable slot-die coating technique, highly ordered Fe2O3 thin films are successfully printed based on the amphiphilic diblock copolymer poly (styrene-b-4-vinyl pyridine) (PS-b-P4VP) as a structure-directing agent. Pure PS-b-P4VP films are printed under the same conditions for comparison. The micellization of the diblock copolymer in the solution, the film formation process of the printed thin films, the homogeneity of the dry films in the lateral and vertical direction as well as the morphological and compositional information of the calcined hybrid PS-b-P4VP/FeCl3 thin film are investigated.

CPP 27.4 Wed 12:15 H39

Morphology transformation pathway of block copolymer- directed cooperative self-assembly of ZnO hybrid films monitored in situ during slot-die coating — •Ting Tian[1], Shanshan Yin[1], Suo Tu[1], Christian L. Weindl[1], Kerstin S. Wienhold[1], Suzhe Liang[1], Matthias Schwartzkopf[2], Stephan V. Roth[2,3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]KTH, Department of Fibre and Polymer Technology, 10044 Stockholm, Sweden — [4]MLZ, TU München, 85748 Garching

Co-assembly of diblock copolymers (DBCs) and inorganic precursors that takes inspiration from the rich phase separation behavior of DBCs can enable the realization of a broad spectrum of functional nanostructures with the desired sizes. In a DBC assisted sol*gel chemistry approach with polystyrene-block-poly(ethylene oxide) and ZnO, hybrid films are formed with slot-die coating. In situ GISAXS measurements are performed to investigate the self-assembly and co-assembly process during the film formation. Combining complementary ex situ characterizations, several distinct regimes are differentiated to describe the morphological transformations from the solvent-dispersed to solidified films. The comparison of the assembly pathway evidences that the key step in the establishment of the pure DBC film is the coalescence of spherical micelles toward cylindrical domains. Due to the presence of the precursor, the formation of cylindrical aggregates in the solution is crucial for the structural development of the hybrid film.

CPP 27.5 Wed 12:30 H39

Programmable Luminescent Tags: Utilizing the interplay of room temperature phosphorescence and oxygen as an information storage device — •Tim Achenbach, Max Gmelch, Heidi Thomas, and Sebastian Reineke — Technische Universität Dresden, Germany

By utilizing the interaction between molecular oxygen and the room temperature phosphorescence of organic materials, continuous-wave-readable and sub-second programmable luminescent tags (PLT) can be realized. They are transparent, flexible and provide a resolution of up to 700 dpi. Information is imprinted by illuminating the PLT with UV light through a shadow mask. By heating the PLT, the information can be erased and a new writing cycle can be started again.

The device consists of two layers on a substrate. The functional layer comprises an organic biluminescent emitter doped into a polymer. The second layer is an oxygen barrier layer. After wet processing in air, molecular oxygen is present in the functional layer of the device, quenching the phosphorescence of the emitter. As energy is transferred to the oxygen during this interaction, it is excited to its highly reactive singlet state and binds to its environment. Over time, all molecular oxygen in the illuminated areas undergoes this photoconsumption process, and a phosphorescent pattern in shape of the mask becomes visible. The oxygen barrier becomes more permeable at elevated temperatures, allowing an oxygen refill of the functional layer by heating the device. This resets the device and it can be rewritten after a short cooling phase.

CPP 27.6 Wed 12:45 H39

Spatio-temporal Imaging of Programmable Luminescent Tags reveals Planar Oxygen Diffusion Properties in Polymer Films — •Richard Kantelberg, Tim Achenbach, Anton Kirch, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany

Programmable Luminescent Tags based on oxygen quenched organic room temperature phosphorescence show application potential in UV sensing and re-writable labelling. This work demonstrates, that the concept can also be exploited to resolve oxygen diffusion properties in thin polymer films, which are essential in everyday applications from medical encapsulation to industrial packaging. In contrast to many established methods, the investigated principle comes without the need of complex pressure sensitive setups or vacuum technology and potentially allows high spatial accuracy. The time-resolved tracking of a two-dimensional phosphorescent pattern reveals the in-plane oxygen diffusion coefficient and considers the photoconsumption of oxygen during the measurement. The diffusion coefficients are determined at the representative case of polystyrene glasses with molecular weights between 13 000 and 350 000 g/mol.

CPP 28: Perovskite and Photovoltaics 3

Time: Wednesday 15:00–17:15 Location: H38

CPP 28.1 Wed 15:00 H38

Optically-Induced Long-lived Chirality Memory in the Color Tunable Chiral Lead-Free Semiconductor (R)/(S)-CHEA4Bi2BrxI10-x (x = 0 - 10) — •Shangpu Liu[1], Markus Heindl[1], Natalie Fehn[2], Sebastián Caicedo-Dávila[1], Silva Kronawitter[2], Gregor Kieslich[2], David Egger[1], Aras Kartouzian[2], and Felix Deschler[1] — [1]Walter Schottky Institute and Department of Physics, TUM, Garching, Germany — [2]Catalysis Research Center, TUM, Garching, Germany

Hybrid organic-Inorganic networks that incorporate chiral molecules have attracted great attention due to their potential in semiconductor lighting applications and optical communication. Here we introduce the chiral organic molecules (R/S)-CHEA into bismuth-based structures with an edge-sharing octahedral motif, to synthesize chiral (R/S)-CHEA4Bi2BrxI10-x crystals and thin films. Using single-crystal X-ray diffraction measurements and density-functional theory calculations, we identify crystal and electronic band structures. We investigate the material optical properties and find circular dichroism, which we tune by the bromide-iodide ratio over a wide wavelength range from 300-500 nm. Further, we employ transient absorption spectra and time-correlated single photon counting to investigate charge carrier dynamics, which show long-lived excitations with unexpected optically-induced chirality memory up to 10s of nanosecond timescales. Our demonstration of chirality memory in a color-tunable and chiral lead-free semiconductor opens a new avenue for the discovery of high-performance spintronic materials with optical functionalities.

CPP 28.2 Wed 15:15 H38

Time-Resolved Microwave Conductivity on ionic liquid doped Lead Halide Perovskites — •Patrick Dörflinger[1], Valentin Schmid[1], Yong Ding[2], Mohammad Khaja Nazeeruddin[2], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Group for Molecular Engineering of Functional Materials, Institute of Chemical Sciences and Engineering, EPFL Valais, Sion 1950, Switzerland

In the past decade, perovskite solar cells evolved to one of the most promising photovoltaic materials with steadily rising power conversion efficiencies, now exceeding 25%. Nonetheless, Organolead Halide Perovskites suffer from insufficient long-term stability. Especially the stability under thermal stress is crucial towards commercialization. Ionic liquids as an additive into the precursor solution are candidates to overcome this issue. Besides the increased resistivity against higher temperatures, alterations of important material properties like mobility and lifetime are expected. Therefore, we used Time-Resolved Microwave Conductivity (TRMC) to determine the mobility and lifetime of photo-generated charge carriers in the perovskite layer. In addition, with Steady-State Microwave Conductivity (SSMC) we can provide insights into the predominating recombination pathways. Combined, we investigated the influence of the ionic liquids on the perovskite material properties and gain deeper understanding of the charge carrier dynamics.

CPP 28.3 Wed 15:30 H38

Hidden interfaces: How ferroelastic domain walls affect the charge diffusion in perovskite solar cells — •Ilka M. Hermes[1,2], Andreas Best[2], Kaloian Koynov[2], Hans-Jürgen Butt[2], and Stefan A. L. Weber[2] — [1]Leibniz Institute for Polymer Research Dresden e.V., Dresden, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany

Ferroelastic domains form during phase transitions that change the crystal system. By arranging in domains with alternating unit cell orientation, the material lowers its overall strain. The walls that separate ferroelastic domains typically feature some structural anomalies, which can affect the electronic properties of the crystal by increasing the defect concentration, introducing dopants or forming a local electric polarization via the flexoelectric effect. Here, we explored the implications of ferroelastic domain walls for the photo-carrier transport in methylammonium lead iodide, a solar cell light absorber used in perovskite solar cells. Via correlative spatial and time-resolved photoluminescence microscopy and electromechanical atomic force microscopy, we could link the presence of domain walls to the occurrence of an anisotropic charge diffusion, where charges move faster parallel to domain walls than perpendicular. Moreover, the ferroelastic nature of the domains promises a targeted engineering of the domain wall arrangement using the application of external stress or heat treatments across the material's cubic-tetragonal phase transition: a perpendicular alignment of the domain walls with respect to the extraction layer interfaces should facilitate faster and more efficient charge extraction.

CPP 28.4 Wed 15:45 H38

Degradation mechanisms of perovskite solar cells under vacuum and one atmosphere of nitrogen — •Renjun Guo[1], Wei Chen[1], Lennart K. Reb[1], Manuel A. Scheel[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Technische Universität München, Garching, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany

Extensive studies have focused on improving the operational stability of perovskite solar cells. Only a few studies survey the fundamental degradation mechanisms related to the device performance, and these studies were executed under various experimental conditions. Thus, we investigate the degradation mechanisms of high-efficiency perovskite solar cells under vacuum and a nitrogen atmosphere, as based on the International Summit on Organic Photovoltaic Stability protocols. We use synchrotron radiation-based operando grazing-incidence X-ray scattering methods. Unlike what was seen in previous reports, we find that the perovskite lattice can also experience a lattice shrinkage under operation. Moreover, we reveal that the atmosphere has a paramount influence on phase segregation, lattice distortion, and morphology deformation during operation of mixed cation lead mixed halide perovskite solar cells. This, in turn, degrades the performance of the respective perovskite solar cells. Our discoveries emphasize the importance of different types of inert atmospheres as critical parameters, which must be considered in future scientific studies and the industrial screening of longevity for photovoltaic modules.

CPP 28.5 Wed 16:00 H38

Determination of the Optimum Dead Area Width of Laser-Patterned, Series-Interconnected Perovskite Solar Cells — •Nicolas Otto[1], Christof Schultz[1], Guillermo Farias Basulto[2], Janardan Dagar[3], Markus Fenske[1], Rutger Schlatmann[1,2], Eva Unger[3], and Bert Stegemann[1] — [1]HTW Berlin - University of Applied Sciences, Wilhelminenhofstr. 75A, D-12459 Berlin — [2]HZB für Materialien und Energie, PVcomB, Schwarzschildstr. 3, D-12489 Berlin — [3]HZB für Materialien und

Energie, Young Investigator Group Hybrid Materials Formation and Scaling, Kekuléstraße 5, D-12489 Berlin, Germany

Based on recent work on minimizing the interconnection width of laser patterned perovskite solar cells the optimum dead area width was determined. In order to use the largest possible aperture area, the dead area width should be as small as possible while still providing full electrical functionality. For this purpose the width between the P2 and the P3 scribes was variated ranging from overlapping to pattering with safety area. By also reducing the P1/P2 spacing an optimum dead area width can be achieved. The detailed scribe line characterization was done by optical microscopy imaging, electrical j-V measurements and compositional analyses. Minimodules with three in series connected cells were then produced. The results show that overlapping scribe lines as well as included safety areas cause avoidable electrical losses. Consequently, an optimum is achieved for arranging the scribe lines as closely as possible. In our study an optimal scribe line width of about 230 micrometres was realized.

CPP 28.6 Wed 16:15 H38

Performance of Perovskite and Organic Solar Cells in Space — •Lennart Reb[1], Michael Böhmer[2], Benjamin Predeschly[1], Sebastian Grott[1], Lukas Spanier[1], Christian Weindl[1], Goran Ivandekic[1], Renjun Guo[1], Christoph Dreissigacker[3], Jörg Drescher[3], Roman Gernhäuser[2], Andreas Meyer[3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, Garching, Germany — [2]TU München, Physik-Department, Zentrales Technologielabor, Garching, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für Materialphysik im Weltraum, Köln, Germany — [4]Heinz Maier-Leibnitz-Zentrum, Garching, Germany

Perovskite and organic solar cells have become a hot research topic in the last few years. The lightweight thin-film solar cells exhibit an exceptional power per mass that exceeds their inorganic counterparts by magnitudes, particularly interesting for space applications. Recently, we launched perovskite and organic solar cells to space on a suborbital rocket flight for the first time [1, 2]. The perovskite and organic solar cells operate in space conditions and produce reasonable power per area of up to 14 and 7 mW cm-2, respectively. Here we derive, with a detailed solar irradiation reconstruction, the irradiation-dependent solar cell performance parameter evolutions, and conclude the solar cell efficiency under strong AM0 irradiation. [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.

15 min. break

CPP 28.7 Wed 16:45 H38

Quantum Efficiency Enhancement of Lead-Halide Perovskite Nanocrystal LEDs by Organic Lithium Salt Treatment — •Roshini Jayabalan[1], Tassilo Naujoks[1], Christopher Kirsch[2], Fengshuo Zu[3], Mukundha Mandal[4], Jan Wahl[2], Martin Waibel[1], Andreas Opitz[3], Norbert Koch[3,5], Denis Andrienko[4], Marcus Scheele[2], and Wolfgang Brütting[1] — [1]Universtität Augsburg, 86135 Augsburg, Germany — [2]Universität Tübingen, 72076 Tübingen, Germany — [3]Instiüt für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany — [4]Max Planck Institut für Polymerforschung, 55128 Mainz, Germany — [5]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany

Owing to large specific surface area in lead halide perovskite nanocrystals, surface passivation using ligands is crucial to attain high photoluminescent quantum yield (PLQY). With respect to device fabrication, such passivation methods must also enable balanced charge injection to achieve high efficiency and operational stability. In this regard, this talk will discuss on the results of post-passivation treatment of CsPbBr3 nanocrystals with LiTFSI, an organic lithium salt. The results from such treatment have proven to be propitious for the nanocrystals - yielding higher PLQY, longer exciton lifetime and improved light outcoupling. Consequently, a significant improvement is observed in the devices fabricated using such post post-treated nanoparticles. Lastly, photoelectron spectroscopy and density functional theory modelling is employed to understand the impact of LiTFSI post-treatment on the performance of a perovskite based LED.

CPP 28.8 Wed 17:00 H38

Tunable mesoporous and optoelectronics properties of zinc titanate films using sol-gel technique — •Yanan Li[1], Nian Li[1], Apostolos Vagias[2], and Peter Müller-Buschbaum[1] — [1]Physics Department, Technical University of Munich, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

Mesoporous films consisting of zinc titanate have high potential applications in photocatalysis, solar cells, and sensors due to tailoring their semiconductive properties. In the present work, we investigate the morphologies of mesoporous zinc titanate films obtained by changing the ratio of two inorganic precursors after calcining hybrid films consisting of organic-inorganic materials. The amphiphilic diblock copolymer poly(styrene)-*b*-poly(ethyleneoxide) PS-*b*-PEO self-assembles into core-shell micelles in a mixture of N,N-dimethylformamid/hydrogen chloride playing the role as structure directing template. The inorganic precursors, zinc acetate dehydrate and titanium tetraisopropoxide, are loaded in the micellar shell due to hydrogen bonds between PEO and precursors. We use slot-die and spin-coating methods to prepare hybrid films, and investigate the influence of the different deposition methods on the film morphologies. Moreover, we investigate how mesoporous structures and crystal phases depend on calcination temperatures. The morphologies of the hybrid films are characterized using grazing incidence small-angle X-ray scattering (GISAXS) and scanning electronic microscopy (SEM).

CPP 29: Biomaterials (joint session BP/CPP)

Time: Wednesday 15:00–17:30 Location: H15

Invited Talk CPP 29.1 Wed 15:00 H15

Bottom-up molecular control of biomimetic hydrogels — •Kerstin G. Blank — Johannes Kepler University, Institute of Experimental Physics, Altenberger Str. 69, 4040 Linz, Austria

The development of biomimetic hydrogels has greatly facilitated fundamental studies aimed at understanding cellular mechanosensing and mechanotransduction processes. It is now widely accepted that cells sense the elastic and viscoelastic properties of their surroundings and respond to these properties via a range of different mechanisms. It is still unknown, however, how cells determine these material properties. Hydrogels are usually characterized as bulk samples while cells interact with these materials in a highly localized manner via specific receptor-ligand interactions. It is thus essential to adopt the cellular point of view and establish a link between microscopic and macroscopic material properties. Towards this goal, we utilize biomimetic hydrogels consisting of mechanically characterized synthetic polymers and extracellular matrix-inspired peptides that serve as physical crosslinks. Using selected examples, we show how crosslink thermodynamics, kinetics and mechanics as well as network topology affect the linear and non-linear viscoelastic properties of molecularly programmed hydrogels. In particular, we highlight that both individual crosslink properties and network topology affect network stress relaxation and show how molecular bond rupture correlates with bulk material failure. Our modular hydrogel system allows for tuning different parameters independently and thus serves as an excellent platform for disentangling the roles of different material properties on cellular responses.

CPP 29.2 Wed 15:30 H15

The role of protein constriction in the fission of membrane tubes — •Russell Spencer and Marcus Müller — Georg-August Universität Göttingen, Institute for Theoretical Physics, 37077 Göttingen, Germany

Membrane remodelling, such as fusion and fission, is involved in a variety of basic, cellular processes. When unaided, the free energy barriers for such remodelling can be prohibitively high, so biological systems employ proteins as catalysts. This work investigates the influence of proteins, such as dynamin, which constrict membrane tubes in order to lower the barrier to fission. We are particularly interested in their role in double-membrane fission as it occurs in mitochondrial division. This work employs self-consistent field theory and utilizes the string method to find the Minimum Free Energy Path (MFEP) in order to determine the most likely pathway for the transition. In addition to lowering the free energy barrier, constriction of the tubes also affects the dominant transition pathway. This work explores the interplay between membrane tension and constriction and the effects that these influences have on fission mechanisms of single and double membrane tubes.

CPP 29.3 Wed 15:45 H15

Rate-Independent Hysteretic Energy Dissipation in Collagen Fibrils — Robert Magerle, •Paul Zech, Martin Dehnert, Alexandra Bendixen, and Andreas Otto — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, 09107 Chemnitz, Germany

Nanoindentation data measured with an atomic force microscope on hydrated collagen fibrils above the glass transition, display a rate-independent hysteresis with return point memory. It is caused by the interplay of elastoplastic deformation during tip indentation followed by elastocapillary recovery of the indent during tip retraction. This previously unknown energy dissipation mechanism dominates at slow indentation rates, where viscous friction is negligible. A generic hysteresis model, based on force-distance data measured during one approach-retract cycle, predicts the force (output) for arbitrary indentation trajectories (input). This model describes collagen fibrils' elastic as well as their dissipative nanomechanical properties with high fidelity for a large range of tip velocities and indentation amplitudes.

15 min. break

CPP 29.4 Wed 16:15 H15

Partition complex structure arises from sliding and bridging — •Lara Connolley and Sean Murray — Max Planck Institute for Terrestrial Microbiology, Marburg, Germany

Chromosome segregation is vital for cell replication and in many bacteria is controlled by the ParABS system. A key part of this machinery is the association of ParB proteins to the parS-containing centromeric region to form the partition complex. Despite much work, the formation and structure of this nucleoprotein complex has remained unclear. However, it was recently discovered that CTP binding allows ParB dimers to entrap and slide along the DNA, as well as leading to more efficient condensation through ParB-ParB-mediated DNA bridging. Here, we use stiff polymer simulations to show how these properties of sliding and bridging can explain partition complex formation. We find that dynamic ParB bridges condense the DNA through the formation of two structures, hairpins and helices. In separate stochastic simulations, we show that ParB sliding accurately predicts the experimentally measured multi-peaked binding profile of Caulobacter crescentus, indicating that bridging and other potential roadblocks are sufficiently short-lived that they do not hinder ParB spreading. Indeed, upon coupling the two simulation frameworks into a unified sliding and bridging polymer model, we find that short lived ParB bridges do not hinder ParB sliding from the parS sites, and can reproduce the binding profile of ParB as well as the overall condensation of the nucleoprotein complex. Overall, our model clarifies the mechanism of partition complex formation and predicts its fine structure.

CPP 29.5 Wed 16:30 H15

Single-chain and condensed-state behavior of hnRNPA1 from molecular simulations — •D. Janka Bauer[1], Lukas Stelzl[1,2], and Arash Nikoubashman[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Biocenter, Institute of Molecular Physiology, Johannes Gutenberg University Mainz, Germany

Intrinsically disordered proteins (IDPs) are essential components for the formation of membraneless organelles, which play key functional and regulatory roles within biological systems. These complex assemblies form and dissolve spontaneously over time via liquid-liquid phase separation of IDPs. Mutations in their amino acid sequence can alter their phase behavior, which has been linked to the emergence of cancer and neurodegenerative diseases. In this work, we study the conformations and phase behavior of a low-complexity domain of heterogeneous nuclear ribonucleoprotein A1 (hnRNPA1), using coarse-grained molecular simulations. We systematically analyze how the single-chain and condensed-state behavior are affected by the number of aromatic residues within the examined sequences. We find a significant compaction of the chains and an increase in the critical temperature with increasing number of aromatic residues within the IDPs. Both observations strongly support the hypothesis that aromatic residues play a dominant role for driving condensation, which is further corroborated by a detailed analysis of the intermolecular contacts. By establishing quantitative comparisons to the experimental phase behavior, we start to critically assess the reliability of coarse-grained IDP models.

CPP 29.6 Wed 16:45 H15

Water flow elastography for minimal invasive surgery — •Paul Kalwa and Tilman Schäffer — University of Tübingen, Germany

Mechanical properties of tissue are of great interest for physicians to differentiate healthy from malign tissue, to determine the status or extent of a disease, and to investigate tissue ageing. The measurement of these properties is therefore a helpful tool for diagnosis. Many elastography techniques have been established and are used in medicine today. However, most of these techniques are not applicable in minimal invasive surgery (MIS), because there the size of probes is limited to a few millimeters and the handling is restricted. We introduce water flow elastography, a novel technique that benefits from a small and inexpensive probe. This technique uses a specialized probe to flow pressurized water against the sample surface, thereby inducing a local indentation. The volume of the indentation, which is measured with a flow meter, is used to quantify the Young's modulus with the help of finite element simulations. We measure the Young's modulus of silicone samples and porcine organs and validate the results with a commercial testing machine, finding agreement within 15 %. We also discuss the suitability of this technique for the determination of viscoelastic tissue properties and for the application in endoscopes for MIS in the future.

CPP 29.7 Wed 17:00 H15

Turning the Corner on the Image Method in Linear Elasticity and Low-Reynolds-Number Hydrodynamics — •Tyler Lutz, Lukas Fischer, Sonja Richter, and Andreas Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

In both linear elasticity and low-Reynolds-number hydrodynamics, extensions of the image method—familiar from elementary electrostatics—have been developed to deduce the displacement (resp. velocity) fields arising from point forces applied in the vicinity of a single, flat, infinitely extended boundary. In this work, we assess the applicability of these methods to domains described by multiple, mutually orthogonal boundaries in 2 and 3 dimensions. Already in the case of a single flat boundary, the necessary image forces depend on the specific boundary conditions considered; the images become progressively more complex as one goes from free-slip to no-slip and stress-free surfaces. By iterating the image method for forces near corners or edges, we explicitly show that this method fails to generate a self-consistent image if any more than one boundary is anything other than a free-slip surface. For the situations in which the image method may be successfully applied, we explicitly construct and survey the qualitative features of the point-force Green's function near corners.

CPP 29.8 Wed 17:15 H15

Adsorption of laminin and cellular response of neurons and glial cells on ion implanted titania nanotube scaffolds — •Jan Frenzel[1,2,3], Astrid Kupferer[1,2], Mareike Zink[3], and Stefan G. Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM), Permoserstraße 15, 04318 Leipzig, Germany — [2]Division of Surface Physics, Department of Physics and Earth Sciences, Linnéstraße 5, 04103 Leipzig, Germany — [3]Research Group Biotechnology and Biomedicine, Department of Physics and Earth Sciences, Linnéstraße 5, 04103 Leipzig, Germany

Brain-machine interfaces are used in a wide spectrum of neuroscience, as for time-resolved sensing of neural activities and for tackling neurodegenerative diseases. Currently established cultivation platforms, including cellulose filters, often result in loss of long-term adhesion, rejection reaction and glial scarring or do not allow for electrical contact due to their insulating properties. As we demonstrate, ion implanted titania nanotube scaffolds (TNS) are a promising candidate to overcome these issues, since they combine a high biocompatibility with a sufficient large electrical conductivity. In our experiments, we explain how ion implantation induced changes of surface characteristics affect the adsorption of laminin and the viability and adhesion of neurons and glial cells. We link the hindered laminin adsorption due to implantation to the shrinkage of tube diameter and rise of zeta potential. The stable and high neuron viability on all TNS but suppressed glial cell formation of implanted TNS gives rise for a potential interface material. Funding by SMWK (100331694) is gratefully acknowledged.

CPP 30: 2D Materials 7 (joint session DS/CPP)

Time: Wednesday 15:00–16:00 Location: H17

CPP 30.1 Wed 15:00 H17

Gate-Tunable Helical Currents in Commensurate Topological Insulator/Graphene Heterostructures — •Jonas Kiemle[1,2], Lukas Powalla[3,4], Katharina Polyudov[3,4], Lovish Gulati[3], Maanwinder Singh[1,2], Alexander Holleitner[1,2], Marko Burghard[3,4], and Christoph Kastl[1,2] — [1]Walter Schottky Institut and Physics Department, Technical University of Munich, Garching, Germany — [2]MCQST, München, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [4]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Van der Waals heterostructures made from graphene and three-dimensional topological insulators promise very high electron mobilities, a non-trivial spin texture and a gate-tunability of electronic properties. Here, we explore epitaxially grown interfaces between graphene and the lattice-matched topological insulator Bi_2Te_2Se. For this heterostructure, spin-orbit coupling proximity has been predicted to impart an anisotropic and electronically tunable spin texture. Polarization-resolved second-harmonic generation, Raman spectroscopy, and time-resolved magneto-optic Kerr microscopies are combined to demonstrate that the atomic interfaces align in a commensurate symmetry with characteristic interlayer vibrations. By polarization-resolved photocurrent measurements, we find a circular photogalvanic effect which is drastically enhanced at the Dirac point of the proximitized graphene. We attribute the peculiar gate-tunability to the proximity-induced interfacial spin structure.

CPP 30.2 Wed 15:15 H17

Topological Invariant of Acoustic Phonons in 2D materials — •Gunnar Lange[1], Adrien Bouhon[1], Bartomeu Monserrat[1,2], and Robert-Jan Slager[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Materials Science and Metallurgy, University of Cambridge, UK

2D materials that live in a 3D space display an unusual acoustic phonon mode: the flexural mode. This mode disperses quadratically away from the center of the acoustic Brillouin zone, and corresponds to a flexing of the material out-of-plane. This differs markedly from the linear dispersion displayed by the in-plane modes, and leads to an unusual triple degeneracy at the zone center. This triple degeneracy is enforced by the Nambu-Goldstone theorem, rather than symmetry, as will be discussed. Such band degeneracies frequently have associated topological invariants. For this triple degeneracy, the topological invariant turns out to generically be of quaternionic type (Euler topology), but reduces to a $\mathbb{Z}_2$ invariant under fairly general assumptions. The invariant has important implications for 2D materials grown on a substrate, as it dictates how the bands are split due to the presence of the substrate. This will be discussed in the context of graphene, where the $\mathbb{Z}_2$ invariant turns out to be non-trivial.

This talk is based on: Lange, G. F., Bouhon, A., Monserrat, B., and Slager, R.-J., "Topological continuum charges of acoustic phonons in two dimensions and the Nambu-Goldstone theorem" Phys. Rev. B **105**, 064301 (2022)

CPP 30.3 Wed 15:30 H17

Coupled Bilayer Graphene Quantum Dots — •Angelika Knothe[1,2] and Vladimir Fal'ko[2,3] — [1]Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]National Graphene Institute, University of Manchester, Manchester, UK — [3]Henry Royce Institute for Advanced Materials, University of Manchester, Manchester, UK

Bilayer graphene quantum dots are promising for spin and valley qubits [1,2,3]. A functional quantum information architecture requires scalable multi-qubit systems. We theoretically study electrostatically confined double-dots and few-dot arrays in bilayer graphene. We quantify the inter-dot couplings for different dot parameters such as the field-induced gap, the confinement shape, and the inter-dot distance. This dependence on external parameters allows tuning the dot arrays into different regimes for which we study the extended Hubbard Hamiltonians and identify the spin and valley level structure. Our results will help to advance the use of bilayer graphene quantum dots for quantum technologies.

[1] A. Knothe, L. I. Glazman, V. Fal'ko, New Journal of Physics 24 (4), 043003 (2022)

[2] S. Möller, L. Banszerus, A. Knothe, C. Steiner, E. Icking, S. Trellenkamp, F. Lentz, K. Watanabe, T. Taniguchi, L. Glazman, V. Fal'ko, C. Volk, C. Stampfer, Phys. Rev. Lett. 127, 256802 (2021)

[3] A. Knothe, V. Fal'ko, Phys. Rev. B 101, 235423 (2020)

CPP 30.4 Wed 15:45 H17

Electron cavity optics in bilayer graphene — Lukas Seemann[1], •Angelika Knothe[1], Klaus Richter[2], and Martina Hentschel[1] — [1]Institute of Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Rapid developments in the field of 2D materials and their nanostructures make it possible to trap charge carriers with different dispersions in various confinement geometries with a high degree of control. This progress now allows studying 2D electron optics phenomena enriched by the charge carriers' different electronic and topological properties compared to the photonic case. Here, we theoretically investigate cavities in gapped bilayer graphene employing an approach based on ray-wave correspondence [1]. We identify the influence of the materials' trigonally warped band structure [2] on the fermion optics characteristics that we show to be conveniently tuneable by gate voltages. Similar considerations can be applied to electron optics in other 2D materials.

[1] J.-K. Schrepfer, S. Chen, M.-H. Liu, K. Richter, and M. Hentschel, Phys. Rev. B 104, 155436 (2021)

[2] C. Gold, A. Knothe, A. Kurzmann, A. Garcia-Ruiz, K. Watanabe, T. Taniguchi, V. Fal'ko, K. Ensslin, T. Ihn, Phys. Rev. Lett. 127, 046801 (2021)

CPP 31: Active Matter 4 (joint session DY/BP/CPP)

Time: Wednesday 15:00–17:30 Location: H18

CPP 31.1 Wed 15:00 H18

Clusters and fractals in non-reciprocally 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 widespread in nature. For the specific case of a binary mixture of passive particles, the breaking of the action reaction principle can lead to formation of active colloidal molecules which are capable of self-propulsion. For small systems, such active molecules have already been realized in experiments based on phoretically interacting binary colloidal mixtures [1,2].

The focus of the present work is to understand the many body behaviour of active molecules. Using particle based simulations and continuum theory, we find that non-reciprocal attractions in a binary mixture of non-motile particles can destabilize the uniform disordered phase and lead to clusters which grow in 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 an effective screening effect which hinges on the characteristic spatiotemporal organization of the two species within the clusters. In addition, remarkably, in a different parameter regime, we find porous macroclusters featuring significant holes and a fractal dimension which differs from the one expected for conventional diffusion limited aggregation.

[1]F. Schmidt et al. J. Chem. Phys. 150, 094905 (2019)

[2]J. Grauer et al. Nat. Commun. 12, 6005 (2021).

CPP 31.2 Wed 15:15 H18

Analysis of transient dynamics of bioconvection in swimming algae — •Alexander Jarosik, Florian von Rüling, and Alexey Eremin — Otto-von-Guericke Universität, Magdeburg, Germany

Swimming unicellular algae Chlamydomonas reinhardtii exposed to light form intricate hydrodynamic instability patterns called bioconvection. High-density plumes of cells are formed in the top layer, descend to the container's bottom, and rise again to the top. This instability arises from coupling between the gyro- and phototactic behaviour of the cells, their physical properties and the flow. In this work, we analyse the microswimmer's dynamics as a function of the cell density, confinement of the environment and light. The transient behaviour of the plume formation is analysed using the Continuous Wavelet Transformation (CWT). We demonstrate that the plume formation can be controlled by local illumination.

CPP 31.3 Wed 15:30 H18

Optimal turbulent transport in microswimmer suspensions — •Henning Reinken^1, Sabine H. L. Klapp^1, and Michael Wilczek^2 — ^{1}Technische Universität Berlin — ^{2}Universität Bayreuth

Microwsimmer suspensions, a paradigmatic example of an active fluid, self-organize into complex spatio-temporal flow patterns, including regular vortex lattices and mesoscale turbulence. This work investigates the transport properties of these suspensions by tracking the diffusive motion of passive tracers in the turbulent flow. We apply a continuum model for the effective microswimmer velocity field [1,2], where the dynamics is governed by the competition between relaxation to a regular vortex lattice and destabilization by nonlinear advection. Varying the strength of nonlinear advection, we observe two qualitatively different regimes of flow transport that we distinguish with the help of the dimensionless Kubo number K, which compares different time scales. Right above the transition to turbulence, the flow field evolves very slowly ($K \gg 1$) and the spatial vortex structures lead to dominant trapping effects. In contrast, for large advection strength, much faster dynamics ($K \ll 1$) leads to transport properties completely determined by the temporal correlations of the flow. In between ($K \approx 1$), we observe a regime of optimal transport, where the diffusion coefficient reaches a maximum.

[1] Reinken, Klapp, Bär, Heidenreich, Phys. Rev. E **97**, 022613 (2018)
[2] James, Bos, Wilczek, Phys. Rev. Fluids **3**, 061101(R) (2018).

CPP 31.4 Wed 15:45 H18

Interfacial activity dynamics of confined active droplets — •Prashanth Ramesh^{1,2}, Babak Vajdi Hokmabad^1, Arnold J.T.M. Mathijssen^3, Dmitri O. Pushkin^4, and Corinna C. Maass^{1,2} — ^{1}Max Planck Institute for Dynamics and Self-Organization — ^{2}University of Twente — ^{3}University of Pennsylvania — ^{4}University of York

Active emulsions exhibit a complex hydrodynamic mode spectrum driven by chemical advection-diffusion instabilities. We study such an active emulsion consisting of oil droplets that dynamically solubilize in a supramicellar aqueous surfactant solution. It has been predicted that the interaction with self-generated chemical fields leads to multistable higher-mode flow fields and chemorepulsive phenomena. To investigate such chemodynamic effects, we study cylindrical droplets pinned between the top and bottom surfaces of a microfluidic reservoir, such that they only produce pumping flows, while we simultaneously quantify the chemical concentration field and the hydrodynamic velocity field. With increasing droplet radius we observe: vortical structures generated by the droplet migrating around the interface, bistability between a dipolar and quadrupolar flow mode, and, eventually, a transition to multipolar modes. We further measured flow fields by particle image velocimetry and compared them to a hydrodynamic model based on a Brinkman squirmer. A simultaneous quantification of the flow fields and oil-filled micelle distribution suggests that a local buildup of chemical products leads to a saturation of the surface, which affects the propulsion mechanism and eventually suppresses all activity.

CPP 31.5 Wed 16:00 H18

Hydrodynamics and fluctuations in bacterial models — •Subhadip Chakraborti — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

Motivated by a biological example of the persistent motion of bacteria, we propose two one-dimensional models of active lattice gases with hardcore interactions. Using macroscopic fluctuation theory (MFT), we analytically derive hydrodynamics for those models and calculate two density-dependent transport coefficients – the bulk-diffusion coefficient and the conductivity, and verify the Einstein relation (ER) by comparing the ratio of those transport coefficients with subsystem number fluctuation. The first model consisting of particles with competing mechanisms of short and long-range hopping obeys the Einstein relation, and exhibits, in the limit of infinite range hopping, upon tuning density (or activity), a 'superfluid' transition from a finitely conducting state to an infinitely conducting one. Interestingly, the bulk-diffusion coefficient remains constant throughout. The diverging conductivity induces 'giant' number fluctuations in the system. In the second model, consisting of hardcore run and tumble particles with persistent motion in one direction decided by an associated spin variable until the direction of spin is reversed, we perform a similar calculation and find that the Einstein relation is violated. This analytic framework could be useful for a better understanding of the collective behavior of many biological systems such as bacterial colonies and other multicellular aggregates, in the context of dynamics and transport properties.

15 min. break

CPP 31.6 Wed 16:30 H18

Shearing an Active Glass — •Rituparno Mandal and Peter Sollich — Institut für Theoretische Physik, Göttingen, Germany

Recent experiments and simulations have revealed glassy features of cytoplasm, tissues and dense assemblies of self propelled colloids. This prompts the fundamental question of whether non-equilibrium (active) amorphous materials are essentially equivalent to their passive counterparts, or whether they can present qualitatively different behaviour. To tackle this challenge we investigate the yielding and mechanical behaviour of a model active glass former, a Kob-Andersen glass in two dimensions where each particle is driven by a constant propulsion force whose direction varies diffusively over time. Using extensive Molecular Dynamics simulations, we focus in particular on the effects of the intermittent dynamics in the regime of highly persistent activity and reveal a novel type of shear induced orientational ordering in the system.

CPP 31.7 Wed 16:45 H18

Active motion with varying self propulsion — Lorenzo Caprini^1, Alexander R. Sprenger^1, Umberto M. B. Marconi^2, Hartmut Löwen^1, and •René Wittmann^1 — ^{1}Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Germany — ^{2}School of Sciences and Technology, University of Camerino, Italy

Active Brownian Particles (ABPs), commonly perceived as the standard model for (dry) active motion, are characterized by a constant self-propulsion velocity along the direction of a unit vector which performs rotational diffusion. In nature, however, the swim velocity is usually not a constant in time and space. Here, we present a generic form of the equations of motion of active particles, which account for two aspects of varying self propulsion. First, we introduce a general stochastic process with fluctuating modulus of the self-propulsion vector, which defines a parental active model (PAM). We argue that the two well-known models of ABPs and Active Ornstein-Uhlenbeck Particles (AOUPs) emerge as limiting cases of the PAM [1], i.e., they are rather sisters than cousins. Second, we demonstrate that a position-dependent swim-velocity field can be consistently introduced for any self-propulsion mechanism [2]. Finally, we discuss the effects of varying self propulsion in external confinement [1,3] and predict the stationary probability distributions in terms of effective interactions [3].

[1] L. Caprini et al., J. Chem. Phys. 156, 071102 (2022).
[2] L. Caprini et al., Soft Matter, 18, 1412 (2022).
[3] L. Caprini et al., arXiv:2203.00603 (2022).

CPP 31.8 Wed 17:00 H18

Perturbing the athermal jamming transition by activity — •Michael Schmiedeberg — Friedrich-Alexander-Universität Erlangen-Nürnberg, 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 three dimensions [1]. We consider the jamming of active particles where the activity corresponds to a perturbation to the athermal jamming process. We find that due to the activity the transition becomes continuous and the transition packing fraction might occur at a different density [2]. The critical exponents agree to those of the universality class of directed percolation. As a consequence, athermal jamming of passive particles seems to be a (singular) limit of the jamming transition in an active system. Note that other perturbation like thermal fluctuations lead to a similar behavior [3]. Therefore, athermal active particles can be seen as a prototype system that leads to new insights how jamming with perturbations (as also studied in [2-5]) can be related to glassy dynamics.

[1] C.S. O'Hern et al., Phys. Rev. Lett. 88, 075507 (2002) and Phys. Rev. E 68, 011306 (2003).

[2] M. Maiti and M. Schmiedeberg, EPL 126, 46002 (2019).

[3] M. Maiti and M. Schmiedeberg, Scientific Reports 8, 1837 (2018); for 2D: Eur. Phys. J. E 42, 38 (2019).

[4] L. Milz and M. Schmiedeberg, Phys. Rev. E 88, 062308 (2013).

[5] S. Wilken et al., Phys. Rev. Lett. 127, 038002 (2021).

CPP 31.9 Wed 17:15 H18

Non-equilibrium phase separation in mixtures of catalytically active particles: size dispersity and screening effects — •Vincent Ouazan-Reboul[1], Jaime Agudo-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK

Biomolecular condensates in cells are often rich in catalytically active enzymes. This is particularly true in the case of the large enzymatic complexes known as metabolons, which contain different enzymes that participate in the same catalytic pathway. One possible explanation for this self-organization is the combination of the catalytic activity of the enzymes and a chemotactic response to gradients of their substrate, which leads to a substrate-mediated effective interaction between enzymes. These interactions constitute a purely non-equilibrium effect and show exotic features such as non-reciprocity. Here, we analytically study a model describing the phase separation of a mixture of such catalytically active particles. We show that a Michaelis-Menten-like dependence of the particles' activities manifests itself as a screening of the interactions, and that a mixture of two differently sized active species can exhibit phase separation with transient oscillations. We also derive a rich stability phase diagram for a mixture of two species with both concentration-dependent activity and size dispersity.

CPP 32: Perovskite and Photovoltaics 4 (joint session HL/CPP/KFM)

Time: Wednesday 15:00–18:15 Location: H34

CPP 32.1 Wed 15:00 H34

Electronic structure analysis of the interface of a TiO_2 electron-transport layer with a perovskite $CsPbI_3$ photovoltaic absorption layer — •Amirhossein Bayani[1], Julian Gebhardt[1], and Christian Elsässer[1,2] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstrasse 11, 79108 Freiburg, Germany — [2]Freiburg Materials Research Center (FMF), Albert-Ludwigs-University Freiburg, 79104 Freiburg, Germany

Lead-based hybrid perovskite halides are currently the most promising light absorbing materials to supplement or even replace Si in next generation solar cells. With intensive research of the bulk material properties in recent years, a strong interest emerges in studying the interfaces to the contact layers in order to reach the final boost of solar efficiency in devices. Here, we study the interface of $CsPbI_3$ with TiO_2 as model interface for a perovskite with an electron transport layer. In particular, we investigate the rutile-TiO_2(001)[001] / $CsPbI_3$(001)[100] interface using self-energy corrected density functional theory. By this state-of-the art modeling technique, we analyze the alignment of workfunctions and investigate the band alignment at the interface.

CPP 32.2 Wed 15:15 H34

Influence of the Ionic Liquid $BMIMBF_4$ on the film formation and optoelectronic properties of $MAPbI_3$ — •Simon Biberger, Konstantin Schötz, Philipp Ramming, Nico Leupold, Ralf Moos, Anna Köhler, Helen Grüninger, and Fabian Panzer — University of Bayreuth, Bayreuth, Germany

Today, metal halide perovskite solar cells (PSCs) are one of the most promising emerging photovoltaic technologies. However, their still limited stability is a main hurdle for their successful commercialization. In the past, various approaches have been developed to improve the long-term stability and performance of PSCs. Here ionic liquids (IL) as additives have attracted much attention as they passivate defects and suppress ion migration. In this work, we investigate the effect of the IL $BMIMBF_4$ on the film formation and optoelectronic properties of the model halide perovskite $MAPbI_3$. By multimodal in situ optical spectroscopy, we investigate the formation of the perovskite film during solution processing via one-step spin coating and a solvent engineering approach and how the film formation alters when the IL is added to the precursor solution. We find that the IL does not impact the formation of perovskite-solvent complexes, but the perovskite growth rate decreases with increasing IL content in the precursor solution. Additionally, we reveal that the IL already interacts with precursor materials and changes the evolution of the PbI_4^{2-} properties. Thus, our work provides important insights into how decisive ILs impact the sensitive interconnection between precursor properties, film formation process and final optoelectronic functionality of perovskite thin films.

CPP 32.3 Wed 15:30 H34

Transversal halide motion enables sharp optical absorption profiles in halide perovskites — •Sebastián Caicedo-Dávila, Christian Gehrmann, Xiangzhou Zhu, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Despite their strong vibrational anharmonicity, halide perovskites (HaPs) exhibit favorable optoelectronic properties, which facilitate their outstanding performance in solar cells, comparable to high-quality inorganic semiconductors. In this contribution, we explore the mechanisms and consequences of dynamic structural flexibility in $CsPbBr_3$ using first-principles molecular dynamics based on density-functional theory. We show that large Br displacements occur on planes that are transversal to the Pb-Br-Pb bonding axis. This *transversality* is concurrent with vibrational anharmonicity, results in short-ranged disorder correlations, and sharpens the joint-density of states rise at finite temperature. Finally, we contrast these results to the case of PbTe, which shares key properties with $CsPbBr_3$ but cannot exhibit any *transversality*, to show that this system features wider band-edge distributions and longer-ranged disorder correlations. These findings are relevant for connecting the structural flexibility and bonding of the halide perovskite structure with the sharp optical absorption of these materials.

CPP 32.4 Wed 15:45 H34

Investigating underlying mechanisms of K doping on stability of single- and mixed-cation perovskite solar cells with experimental and computational informed modelling — Saied Mollavali, Mohammad Moaddeli, and •Mansour Kanani — Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran

Recent studies revealed that the interstitial occupancy of potassium in single/mixed-cation based perovskite structures could hinder the ion migration mechanisms near interfaces, and therefore leads to a better structural stability. However, the underlying stability enhancement mechanisms and probable side effects of additional K atoms in corporate with other organic/inorganic constituents, with a long-range electronic bonding character, is not clear completely. In this study, the effect of doping K on the structural, morphological, electronic, and optical properties of different perovskite structures is investigated experimentally and computationally. The beneficial effect of interstitial K atom on long-range bonding of I atoms with organic molecules is observed. Furthermore, no degradation from additional K is detected for specific range of doping. This result opens a new insight on constructive impact of inorganic dopant on stability issue in perovskite solar cells. SEM, XRD, Photoluminescence and optical absorbance analysis were performed on the perovskite layer. The one layer-based experimental data incorporation with DFT based results were informed into the SCAPS-1D solar cell simulator package to predict cell efficiency, systematically.

CPP 32.5 Wed 16:00 H34

Revealing efficiency losses due to mobile ions in perovskite solar cells — •Sahil Shah, Jarla Thiesbrummel, and Jonas Diekmann — University of Potsdam, Germany

Perovskite semiconductors are distinct from most other semiconductors due to a large number of mobile ions in the active layer (e.g., iodide and methylammonium ions and vacancies, and others). Thus, ion dynamics have a critical impact on the performance and stability of perovskite-based applications.

In this work, we will show how the ionic density and induced losses change with device degradation under elevated temperatures and continuous light illumination. This is investigated via a simple and newly developed method *fast-hysteresis* which is a JV scan at a faster rate (˜1000 Vs-1) which prevents the perturbation of mobile ions and we get the true ion free potential of the device. The fast-hysteresis measurements are corroborated by transient charge extraction and capacitance measurements as well as numerical simulations, which provide important insights into the dynamics of free electronic charges and mobile ions. We will then demonstrate how the mobile ions affect a range of commonly used mixed cation metal halide perovskite compositions and how the ionic losses vary with the charge transport layer.

Overall, the proposed methods quantify the ion-induced field screening, shed light on the complex device degradation process and PCE losses allow for a better understanding of several key phenomena in perovskite solar cells, and open up a large range of future experiments.

CPP 32.6 Wed 16:15 H34

Dissecting Ultrafast Polarization Responses in Lead Halide Perovskites via the THz-induced Kerr Effect — •Maximilian Frenzel[1], Marie Cherasse[1,2], Joanna Urban[1], Feifan Wang[3], Bo Xiang[3], Leona Nest[1], Lucas Huber[3], Martin Wolf[1], X.-Y. Zhu[3], and Sebastian F. Maehrlein[1] — [1]Fritz Haber Institute of the Max Planck Society, Department of Physical Chemistry, Berlin, Germany — [2]LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France — [3]Columbia University, Department of Chemistry, New York City, USA

The microscopic origin of the surprising optoelectronic properties of lead halide perovskite (LHP) semiconductors is still under debate. One hypothesis is that the highly polar and anharmonic lattice of LHPs influences their optoelectronic properties through dynamic charge carrier screening. We therefore study the ultrafast polarization response of the hybrid LHP MAPbBr$_3$ when exposed to transient electric fields in the form of intense, single-cycle THz pulses. By probing the THz-induced Kerr effect (TKE), we observe strong THz polarizability and complex ultrafast polarization dynamics. We perform 4-wave-mixing simulations, which show that it is crucial to account for anisotropic and dispersive light propagation for the correct interpretation of the measured TKE signals. Finally, we unveil a coherent phonon response in MAPbBr$_3$, which we assign to the inorganic cage and conclude to be the dominating polarizable mode in this material. This finding highlights the role of the inorganic lattice for dynamic carrier screening and the related mechanism of charge carrier protection.

30 min. break

CPP 32.7 Wed 17:00 H34

Calculating the temperature-dependent band gap of the halide perovskite CsPbBr$_3$ — •Stefan Seidl, Christian Gehrmann, Xiangzhou Zhu, Sebastian Caicedo Davila, and David A. Egger — Department of Physics, Technical University of Munich, Garching, Germany

Theoretical calculations based on density functional theory (DFT) can predict thermal effects in the electronic structure by considering important phenomena, such as thermal lattice expansion and electron-phonon coupling. The latter can be calculated using a Monte-Carlo (MC) sampling approach that is formally rooted within the harmonic approximation, which has recently been shown to yield accurate temperature-dependent band gaps for inorganic semiconductors [1]. A complementary approach to predict thermal effects in the electronic structure is first-principles molecular dynamics (MD), which can account for vibrational anharmonicity that is an important effect for certain technologically relevant materials. Here, we assess the temperature-dependent band gap of the halide perovskite CsPbBr$_3$ in the cubic and orthorhombic phases employing the two different methods, MC and MD, and compare our findings with experimental results. This includes a discussion about the role of anharmonicity and the contributions from spin-orbit coupling and thermal lattice expansion.

[1] F. Karsai et al, New J. Phys. 20, 123008 (2018)

CPP 32.8 Wed 17:15 H34

Electronic structure prediction of hybrid organic-inorganic metal halide perovskites using cost-effective DFT-1/2 method — Mohammad Moaddeli und •Mansour Kanani — Department of Materials Science and Engineering, School of Engineering, Shiraz University, Shiraz, Iran

Hybrid organic-inorganic metal halide perovskites (OIHPs) have attracted much attention in the last decade because of tunable photovoltaic performance and low fabrication cost. Regarding the tunable parameters for controlling the fundamental properties of OIHPs, recent computational and data-driven based approaches can accelerate new material prediction procedure significantly. Density functional theory (DFT) is considered as fundamental block of many multiscale, high-throughput and data-driven approaches typically. However, because of complexity of electronic orbital in OIHP as well as high sensitivity of regarding properties to atomistic configuration, employing conventional computational approaches faces many obstacles or needs very expensive corrections. Underestimation of routine functionals used in DFT calculations push people apply expensive approaches such as hybrid functionals and GW approximation. Here, DFT-1/2 method with a normal computational cost has been used for determining not only the band gap but also the true form of valence and conduction bands of OIHPs. The results showed that, the method could preserve the known Rashba band splitting in the conduction band of mixed-cation perovskites, which is the source of longer carrier lifetime behavior.

CPP 32.9 Wed 17:30 H34

Phonon Signatures for Polaron Formation in an Anharmonic Semiconductor — •Feifan Wang[1,2], Weibin Chu[3], Jin Zhao[3], and X.-Y. Zhu[1] — [1]Columbia University, New York, NY, 10027 USA — [2]Dept. of Materials, ETH Zurich, Switzerland — [3]University of Science and Technology of China, Hefei, Anhui 230026, China

Polaron formation, in which charge carriers are dressed by a cloud of lattice distortions, is partially responsible for the long carrier lifetimes and diffusion lengths in the lead halide perovskite (LHP), a superior optoelectronic material. Considerations of ferroelectric-like phonon anharmonicities of this system lead to the recent proposal of ferroelectric large polarons, which attributes efficient charge-carrier screening to the extended ordering of dipoles associated with inversion-symmetry-breaking unit cells. Here, we study electron-phonon coupling in Bi$_2$O$_2$Se, a semiconductor which bears resemblance to LHPs in ionic bonding, band transport with long carrier diffusion lengths, and dynamical phonon disorder as revealed by low-frequency Raman spectroscopy. Using coherent phonon spectroscopy, we show the strong coupling of an anharmonic phonon mode to photo-excited charge carriers, while the Raman excitation of this mode is symmetry-forbidden in the ground-state. Density functional theory calculations verify that the phonon mode originates from the symmetry reduction after charge injection and indicate the local dipole ordering induced by photo-excited electrons. This study provides an initial attempt to generalize the proposed charge-carrier screening model to account for the outstanding optoelectronic properties of defect-tolerant semiconductors.

CPP 32.10 Wed 17:45 H34

Tuning Perovskite Crystallization in the Hybrid Route — •Mohamed Mahmoud, Patricia Schulze, Andreas Bett, and Oussama Er-raji — Fraunhofer ISE

In 2009, perovskite solar cells were discovered in the solid-state that can be used not only as a single junction absorber but also in tandem configuration thanks to their bandgap tunability. It is a combination of organic and inorganic lead halide materials and they have the advantage of a strong absorption edge, defect tolerance and potential cheap production due to easy production methods such as spin coating or slot-die coating as a highly scalable production method. In the industry, double-sided textured silicon (DSTS) is commonly produced to overcome the reflection losses at surfaces. Spin coating of perovskite on top of DSTS resulted in low conformality which resulted in shunts and non-working solar cells. To overcome this issue, the hybrid route was developed, in which inorganic materials are co-evaporated using the thermal vapour deposition technique and then organic materials are spin-coated. By doing that, the high conformality of the thin film on top of the c-Si is achieved. However, the resulting perovskite grain size is in the nanometer scale. To increase the grain size - which results in higher short circuit current, lower grain boundaries and thus a more stable device - thermodynamics of the crystallization process need to be studied. In this work, using the thermodynamics fundamentals of crystallization, we tune the grain size of perovskite deposited via the hybrid route. In addition, we study the consequences of different grain sizes on the efficiency of the solar cell and especially on the stability.

CPP 32.11 Wed 18:00 H34

Dynamic nuclear spin polarization in lead halide perovskites — •Natalia Kopteva[1], Dennis Kudlacik[1], Marek Karzel[1], Mladen Kotur[1], Dmitri Yakovlev[1], Oleh Hordiichuk[2], Olga Nazarenko[2], Dmitry Dirin[2], Maksym Kovalenko[2,3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, TU Dortmund, 44221 Dortmund, Germany — [2]Laboratory of Inorganic Chemistry Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics Empa-Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Lead halide perovskites are promising for applications in spintronics due to the nanosecond coherence time of the resident carriers [1]. The primary source of losing spin coherence is the interaction with the fluctuating nuclear spin environment [2]. Optically oriented carrier spins polarize nuclei, which create an Overhauser field. Due to the different strengths of the hyperfine interaction with the nuclear spins, the electron and hole experience different magnitude and directions of the Overhauser field. To study the degree of nuclear spin polarization and fluctuation, we investigate the interaction of resident and optically created carrier spins with nuclei using the Hanle effect in the tilted magnetic field in bulk formamidinium caesium lead iodine bromide.

[1] V. V. Belykh et al., Nat. Commun. 10, 673 (2019)

[2] I. A. Merkulov et al., Phys. Rev. B 65, 205309 (2002)

CPP 33: Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 1

organized by Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TUM) and Walter Richtering (RWTH Aachen)

Time: Thursday 9:30–11:15 Location: H38

Invited Talk CPP 33.1 Thu 9:30 H38

Cooperative and non-Gaussian dynamics of entanglement strands in polymer melts — •Margarita Kruteva[1], Michaela Zamponi[2], Ingo Hoffmann[3], Jürgen Allgaier[1], Lutz Willner[1], Andreas Wischnewski[1], Michael Monkenbusch[1], and Dieter Richter[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1: Neutron Scattering and Biological Matter), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstraße 1, 85748 Garching, Germany — [3]Institut Laue-Langevin (ILL), B.P. 156, F-38042 Grenoble Cedex 9, France

We report neutron spin echo investigations on the motion of short tracer chains in highly entangled melts [1,2]. The tracers were found to undergo sub-diffusion behavior. Unexpectedly the sub-diffusion is limited by a distance very close to the tube diameter of the respective highly entangled host. The cross-over distance to Fickian diffusion, thereby, is independent of the tracer's length. The Fickian diffusivity agreed with the macroscopic results. We found that the Rouse dynamics of the tracers is strongly non-Gaussian with a related segment displacement distribution narrower than the Gaussian counterpart. These results were understood as a consequence of highly cooperative motion of the tracers with the host that mirrors the host dynamics within the tube. The phenomena were found both in a polyolefin (polyethylene) as well as in a polyether (polyethylene-oxide) indicating their generality. (1) Zamponi, M. et al. Phys. Rev. Lett. 2021, 126 (18), 187801. (2) Kruteva, M. et al. Macromolecules 2021, accepted.

CPP 33.2 Thu 10:00 H38

Molecular weight dependent dynamics of polymers grafted on nanoparticles. — •Aakash Sharma[1], Margarita Kruteva[1], Michaela Zamponi[2], Sascha Ehlert[1], Dieter Richter[1], and Stephan Förster[1] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1: Neutron Scattering and Biological Matter), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstraße 1, 85748 Garching, Germany

Grafting polymer chains on nanoparticles prevents their undesired aggregation leading to improved properties. Whereas, grafting induces inevitable alteration in the dynamics of polymer chains, which affects macroscopic properties e.g. viscoelasticity. It has been established that the polymer chain dynamics is retarded in grafted chains. However, literature lacks consensus on whether the segmental dynamics of grafted chains is accelerated or retarded. We study the segmental dynamics of polyisoprene grafted on spherical nanoparticles using neutron backscattering. The analysis of relaxation times led to the conclusions: (i) Low molecular weight (MW) grafted polymer display reduced local relaxation (ii) At high MW and equal grafting density faster segmental dynamics than the free polymer is observed. We prove that these conflicting results are seemingly artifacts of the traditional analysis method. We invoke an elegant methodology and show that the underlying physics of grafted polymer is unchanged. However, spatial variation of the relaxation times across the grafted chain causes the average dynamics to transition with molecular weight.

CPP 33.3 Thu 10:15 H38

Structure and Dynamics of Polymer Brushes and Microgels at Interfaces measured with Neutron Scattering — •Olaf Holderer[1] and Stefan Wellert[2] — [1]Jülich Centre for Neutron Science at MLZ, Forschungszentrum Jülich GmbH, 85748 Garching, Germany — [2]Department of Chemistry, Technische Universität Berlin, 10623 Berlin, Germany

It is an experimental challenge to access structural and dynamic properties of brushes and microgels at the solid liquid interface [1]. Neutron scattering techniques such as Grazing Incidence Small Angle Neutron Scattering (GISANS) for structural investigations and Grazing Incidence Neutron Spin Echo Spectroscopy (GINSES) provide a means of studying structural and dynamic properties on molecular length scales at the interface. Simulations of the experimental conditions in the framework of the Distorted Wave Born Approximation help interpreting the static and dynamic scattering signals [2]. Examples of thermoresponsive microgels with different architecture and brushes at the interface are presented to illustrate the possibilities and challenges of this type of interface studies.

[1] J. Witte, T. Kyrey, J. Lurtzki, A.M. Dahl, M. Kühnhammer, R. von Klitzing, O. Holderer, S. Wellert, ACS Appl. Polym. Mater. 2021, 3, 2, 976-985

[2] T. Kyrey, M. Ganeva, J. Witte, R. von Klitzing, S. Wellert, O. Holderer, J. Appl. Cryst. (2021) 54, 72-79

CPP 33.4 Thu 10:30 H38

In-situ neutron reflectometry measurements of polyelectrolyte diffusion in Layer-by-Layer films in aqueous solution at ILL — •Annekatrin Sill[1], Heiko Ahrens[1], Olaf Soltwedel[2], Philipp Gutfreund[3], and Christiane A. Helm[1] — [1]University of Greifswald, Institute of Physics, D-17489 Greifswald, Germany — [2]Technische Universität Darmstadt, Institute for Condensed Matter Physics, D-64289 Darmstadt, Germany — [3]Institut Laue-Langevin, F-38042 Grenoble, France

Up to now, we measured vertical polyelectrolyte diffusion in Layer-by-Layer films by immersing the film for a defined amount of time in the annealing solution. Then the film was dried, and a snapshot was taken. With the snapshot method, one can get good results, but we wanted to develop an improved method. For the first time, the dynamics of our films were studied in-situ at the Institut Laue-Langevin (ILL) on instrument D17. This neutron reflectometer with horizontal scattering geometry is suitable for in-situ measurements, using wavelengths from 2 to 27 Å with great flexibility in resolution. We used the slab architecture with selective polyanion deuteration to study vertical polyanion diffusion. As polycation linear PDADMA was used, PSS/PSSd was the polyanion. Each film consisted of a protonated and a deuterated slab. Varied were the salt concentration and the temperature of the annealing solution. The diffusion constant was determined and compared to the snapshot measurements in air.

CPP 33.5 Thu 10:45 H38

Kinetics of mesoglobule formation and dissolution in solutions of thermoresponsive polymers after fast pressure jumps

— Bart-Jan Niebuur[1], Leonardo Chiappisi[2], Alfons Schulte[3], and •Christine M. Papadakis[1] — [1]Technical University of Munich, Physics Department, Garching, Germany — [2]Institut Laue-Langevin, Grenoble, France — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando FL, U.S.A.

The thermoresponsive polymer poly(*N*-isopropylacrylamide) (PNIPAM) features lower critical solution temperature behavior in aqueous solution with the cloud point depending on pressure [1]. Fast pressure jumps across the coexistence line in combination with time-resolved small-angle neutron scattering elucidate the pathways of mesoglobule formation and disintegration over a wide range of length scales with a time resolution of 50 milliseconds. Varying the start and target pressures gives insight into the role of thermodynamic and kinetic factors governing mesoglobule formation [2,3]. For disintegration, the osmotic pressure of the solvent within the mesoglobules is the decisive factor for the mechanism and the time scales [4]. These results are of importance for applications of thermoresponsive polymers as switches. 1. B.-J. Niebuur et al., ACS Macro Lett. 6, 1180 (2017). 2. B.-J. Niebuur et al., ACS Macro Lett. 7, 1155 (2018). 3. B.-J. Niebuur et al., Macromolecules 52, 6416 (2019). 4. B.-J. Niebuur et al., RSC Nanoscale 13, 13421 (2021).

CPP 33.6 Thu 11:00 H38

Simultaneous SAXS/SANS method: A novel nanoanalytical tool — •Ezzeldin Metwalli[1], Klaus Götz[1], Tobias Zech[1], Christian Bär[1], Anne Martel[2], Lionel Porcar[2], and Tobias Unruh[1] — [1]Institute for Crystallography and Structural Physics (ICSP), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — [2]Institut Laue-Langevin, 71, Avenue des Martyrs, Grenoble, 38042, France

Exploiting X-ray and neutron beams at the same sample volume enables unprecedented investigations of nanomaterials using small angle scattering (SAS) technique. A portable small angle X-ray scattering (SAXS) instrument with a proper geometrical dimension was successfully designed, constructed and implemented at D22 zone of Institut Laue Langevin (ILL) in France for simultaneous SAXS/SANS experiments. Compared with an independent experimental approach, the simultaneous SAXS/SANS experimental approach ensures the exactness of the probed samples, especially for time-resolved studies. The SAXS/SANS experimental setup will indispensably permit to instantaneously analyse and understand the complicated correlated nanostructures of two different types of nanoscale components in the same sample volume. For instance, a temporal structural cross-correlation between organic stabilizing agent (cetyltrimethylammonium bromide; CTAB micelles) and gold seeds, which cooperate in the formation of different size/shape of large stabilized gold nanorods during the synthesis process [1] was successfully probed. [1] T. Zech, et.al., Part Part Syst Charact, 39, 2100172, 2022.

CPP 34: Hydrogels and Microgels

Time: Thursday 9:30–10:15 Location: H39

CPP 34.1 Thu 9:30 H39

Simulations explain the Swelling Behavior of Hydrogels with Alternating Neutral and Weakly Acidic Blocks — •David Beyer[1], Peter Košovan[2], and Christian Holm[1] — [1]Institute for Computational Physics, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Department of Physical and Macromolecular Chemistry, Charles University, Prague, Czechia

We use computer simulations to study a coarse-grained model of a weak (pH-responsive) polyelectrolyte hydrogel which consists of a covalent, regular tetra-functional network of four-armed neutral and acidic stars, coupled to a reservoir of small ions. A similar system consisting of tetrapoly-(acrylic acid) and tetrapoly(ethylene glycol) was recently investigated experimentally by the Sakai group. To model the ionization equilibrium of the weak groups and the exchange of small ions with the reservoir, we make use of the recently developed Grand-Reaction Monte-Carlo method (G-RxMC). We determine the free swelling equilibrium for different salt concentrations and pH values of the reservoir. The results for the swelling ratio are in good agreement with the experimental data for high and intermediate pH values. We obtain titration curves which display a significant deviation from the ideal Henderson-Hasselbalch equation due to charge correlations and Donnan partitioning. Contrary to a previous conjecture, our results show that counterion condensation does not explain the observed swelling behavior. Finally, we investigate the gel structure and observe that the swelling is dominated by the stretching of the acidic blocks.

CPP 34.2 Thu 9:45 H39

Importance of pH in Synthesis of pH-Responsive Cationic Nano- and Microgels — •Marco Annegarn, Maxim Dirksen, and Thomas Hellweg — Department of Physical and Biophysical Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

While cationic nano- and microgels are potentially useful for transfection of cells or the immobilization of biomacromolecules, their synthesis often has certain drawbacks regarding size, polydispersity, yield and incorporation of the cationic comonomer. Since many cationic comonomers like primary or secondary amines are pH-responsive, their charge relies on the surrounding pH. Therefore, a range of poly(*N*-isopropylacrylamide) (PNIPAM) microgels with the primary amine *N*-(3-aminopropyl)methacrylamide hydrochloride (APMH) as the cationic comonomer were synthesized at different reaction pH. The microgels were analyzed with respect to their size, thermoresponsive swelling behavior, synthesis yield, polydispersity and APMH-incorporation.

The results show that the reaction pH has a strong influence on on all the mentioned parameters and can be utilized to tailor the microgels properties. While the influence of the pH on such microgels has been examined repeatedly after synthesis, the influence of the reaction pH during synthesis is mostly ignored. Hence, a precise pH-control during the synthesis of microgels with pH-responsive moieties is crucial to gain reproducible and comparable results.

CPP 34.3 Thu 10:00 H39

Behaviour of a magnetic nanogel in a shear flow — •Ivan Novikau[1], Ekaterina Novak[2], Elena Pyanzina[2], and Sofia Kantorovich[1,2] — [1]University of Vienna, Austria — [2]Russia

Magnetic nanogels (MNG) are promising magneto-controllable drug carriers. In order to develop this potential, one needs to study MNG's behavior in various microfluidic systems, one of which can be modelled as a channel with a given flow.

Considering the size of the MNG and typical time and velocity scales involved in their nanofluidics, experimental characterisation of the system is challenging. In this work, we perform molecular dynamics (MD) simulations combined with the Lattice-Boltzmann (LB) scheme aiming at describing the impact of the shear rate on the shape, magnetic structure and motion of an MNG.

We find that in a shear flow, the centre of mass of an MNG tends to be in the centre of a channel and to move, preserving the distance to both walls. The MNG monomers along with translation are involved in two more types of motion, they rotate around the centre of mass and oscillate with respect to the latter. It results in synchronised tumbling and wobbling of the whole MNG accompanied by its volume oscillates. We show that the volume oscillations and rotations are two faces of the same periodic process whose frequency is a growing function of the shear rate and depends on strength of magnetic interaction between magnetic nanoparticles. We demonstrate that the oscillations of the volume lead to the periodic changes in MNG magnetic energy.

CPP 35: 2D Materials 8 (joint session DS/CPP)

Time: Thursday 9:30–11:30 Location: H17

CPP 35.1 Thu 9:30 H17

Calculation of Elastic Properties in Monolayer Covalent-Organic Frameworks — •David Bodesheim[1], Antonios Raptakis[1], Jonathan Heinze[1], Arezoo Dianat[1], Robert Biele[1], Alexander Croy[2], and Gianaurelio Cuniberti[1] — [1]TU Dresden, Dresden, Germany — [2]FSU Jena, Jena, Germany

Covalent-Organic Frameworks (COFs) are crystalline porous materials that are based on organic monomeric units, so called building blocks. Through recent experimental progress, mono- and few-layer COF materials have been synthesized, providing a new class of 2D materials.[1,2] From a computational point of view, however, accurately calculating properties of these materials is demanding as their unit cells are usually very big. In this work, we calculate elastic properties for a multitude of 2D COFs in a high-throughput manner. The calculations are based on classical force-fields and are compared with higher level of theory like density functional based tight binding (DFTB). We show how force-fields can be very useful for mechanical property calculation, how their accuracy can be improved, and typical fallacies for 2D COFs. Furthermore, we introduce models to predict mechanical properties from the properties of their monomeric building blocks.[3] This paves the way for accurate multiscale modeling, high-throughput calculations, and materials design with properties on demand.

[1] A. Ortega-Guerrero, et al. ACS Appl. Mater. Interfaces, 13, 22, 26411-26420 (2021).

[3] Z. Wang, et al., Nat. Synth., 1, 69-76 (2022).

[3] A. Raptakis, et al. Nanoscale, 13, 1077 (2021).

CPP 35.2 Thu 9:45 H17

Light-Matter Interaction in 2D Polar Metals — •Margaux Lassaunière[1], Wen He[2], Katharina Nisi[1], Shruti Subramanian[3], Siavash Rajabpour[3], Alexander Vera[3], Nathalie Briggs[3], Su Ying Quek[2], Joshua Robinson[3], and Ursula Wurstbauer[1] — [1]Institut of Physics, Münster University, Germany — [2]Department of Physics, National University of Singapore, Singapore — [3]MatSE; Center for 2DLM; ATOMIC; 2D Crystal Consort.; Penn State University, USA

Understanding and controlling the light-matter interaction in thin metal films is of high technological relevance. Here, we study the linear optical response of atomically thin 2D gallium, 2D indium as well as their alloys embedded in half-van der Waals heterostructures by spectroscopic imaging ellipsometry. The thin films are prepared via confinement heteroepitaxy (Chet). In a systematic study of the dielectric functions, we separate free and bound electron contributions to the optical response, with the latter pointing towards the existence of thickness-dependent quantum confinement phenomena and epsilon near zero (ENZ) behaviour [1]. The resonance energies of the observed ENZ behaviour are dependent on the number of atomic metal layers, materials, and alloying [2]. Their tunability makes 2D polar metals attractive for quantum engineered metal films, tunable (quantum-)plasmonics and nano-photonics.

[1] K. Nisi et al. Adv. Mater. 2021, 2104265

[2] S. Rajabpour et al. Adv. Funct. Mater. 2020, 2005977

CPP 35.3 Thu 10:00 H17

Layer dependent anisotropic dielectric function of the magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Margaux Lassaunière[1], Julian Klein[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology, USA

The van der Waals (vdW) material CrSBr is a 2D magnetic semiconductor with ferromagnetic ordering within each layer. Adjacent layers, however, are coupled antiferromagnetically. As a vdw semiconductor with a direct band gap, the light matter interaction is determined by strong excitonic resonances that are highly anisotropic in the crystal plane. We experimentally determine the complex dielectric function in the near infrared to visible regime along the two main crystal directions by spectroscopic imaging ellipsometry (SIE) measurements and regression analysis to a multilayer model. Unlike other vdW semiconductors such as MoS2 or WSe2 [1], the rich excitonic signatures in the dielectric function are highly anisotropic and show only minor distinct dependence on the number of layers. Even more striking, we find that the excitonic resonance are better pronounced for multilayer compared to monolayer CrSBr with significantly reduced line-width even at room temperature. [1] Wurstbauer et al. J. Phys. D: Appl. Phys. 50, 173001 (2017).

CPP 35.4 Thu 10:15 H17

Tracing the Superconducting Phase Transition in Atomically Thin 2D Polar Gallium by Transport and Spectroscopic Ellipsometry — •Jakob Henz[1], Margaux Lassunière[1], Pierre-Maurice Piel[1], Siavash Rajabpour[2], Alexander Vera[2], Joshua Robinson[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]MatSE; Center for 2DLM; Atomic; 2D Crystal Consort, PennState University, USA

Half van der Waals 2D polar metals are a novel class of 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms such as gallium or indium are intercalated between graphene and a silicon carbide substrate. This results in large area, environmentally stable, 2D metals with a bonding gradient in z-direction ranging from covalent over metallic to vdW within only two to three atomic layers. The materials feature interesting properties such as superconductivity[1] and a large plasmonic response in the visible range[2]. 2D gallium is studied by temperature dependent spectroscopic ellipsometry and transport measurements down to below 1K. We extract the dielectric function in the visible to near infrared range with a special focus on signatures across the phase transition from metallic to superconducting behavior unambiguously identified from the abrupt drop in the temperature dependent sheet resistance at the transition temperature T_C of about 3.5 K.

1 S. Rajabpour et al., Adv. Mater. 2104265 (2021)
2 Nisi et al., Adv. Funct. Mater. 2005977, 1-11 (2020)

CPP 35.5 Thu 10:30 H17

Epitaxial growth of $Fe_{5-x}GeTe_2$ films with a Curie temperature above 300 K on graphene — Hua Lv[1], Jens Herfort[1], Jürgen Schubert[2], Michael Hanke[1], Manfred Ramsteiner[1], and •Joao Marcelo J. Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, Germany

Synthesis of magnetic 2D materials exhibiting transition temperatures at or above 300 K is a crucial step towards the development of ultra-compact spintronic devices. Here, we report our recent progress on epitaxial growth of the 2D ferromagnet $Fe_{5-x}GeTe_2$ via MBE on graphene on SiC(0001). Thin films with a thickness of about 10 nm and different Fe concentrations were studied. Characterization performed with methods such as in-situ RHEED and grazing incidence X-ray diffraction confirmed the formation of epitaxial layers with good crystalline quality. Magneto-transport measurements and SQUID magnetometry were employed to assess the electrical and magnetic properties. They reveal that the MBE-grown $Fe_{5-x}GeTe_2$ exhibits a metallic behavior for all investigated Fe concentrations. In addition, composition-dependent magnetic anisotropies and Curie temperatures (T_C) were deduced. For the Fe content close to 5, a predominant easy out-of-plane orientation and T_C well above 300 K were measured. These results are relevant for the further development of wafer-scale fabrication of magnetic 2D materials aiming at the realization of multifunctional, atomically thin devices.

CPP 35.6 Thu 10:45 H17

Antisymmetric magnetoresistance in a Fe_3GeTe_2-Fe_3GeTe_2 van der Waals ferromagnetic homojunction — •Jan Bärenfänger[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jonathan Eroms[1], Dieter Weiss[1], and Mariusz Ciorga[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan

The emergence of novel two-dimensional (2D) magnetic van der Waals (vdW) materials have breathed new life into the field of spintronics. The weak vdW interaction between layers of strong covalent bonds enables the exfoliation of these materials down to monolayers. Furthermore, vdW heterostructures can easily be fabricated by stacking them on top of each other like LEGO blocks, bringing a platform for novel spintronic devices. Here, we report an antisymmetric magnetoresistance (MR) in an Fe3GeTe2- Fe3GeTe2 (FGT) vdW homojunction. We attribute it to eddy currents emerging at the interface of the antiparallel, perpendicular-to-plane magnetized FGT flakes, due to the different sign of the anomalous Hall effect in both flakes. These eddy currents perturb the measured longitudinal resistance, resulting in the observed antisymmetry. Such an interpretation is supported by the observation of a sign change of the MR when measuring the voltage drop along the opposite edges of the transport channel . This work highlights the potential for new spintronic applications using vdW ferromagnets.

CPP 35.7 Thu 11:00 H17

Charge-transfer stabilization, modulation doping, and CDW phase in layered ferecrystal heterostructures — •Fabian Göhler[1], Shrinidhi Ramasubramanian[1], Sanam K. Rajak[1], Niels Rösch[1], Adrian Schütze[1], Susanne Wolff[1], Marisa Choffel[2], Dmitri L. M. Cordova[2], David C. Johnson[2], and Thomas Seyller[1] — [1]Chemitz University of Technology, 09126 Chemnitz, Germany — [2]University of Oregon, Eugene 97403, USA

A virtually unlimited number of metastable, layered heterostructures - called *ferecrystals* due to the non-epitaxial alignment between layers - can be grown via the self-assembly of layered amorphous precursors. [1] In this contribution, we want to highlight recent investigations on the electronic structure and interlayer interactions in several series of compounds using photoemission spectroscopy (PES).

In the Bi-Mo-Se system, the formation of the metallic 1T-polytype of MoSe$_2$ is aided by charge transfer from rock-salt structured BiSe. By systematically stacking BiSe, Bi$_2$Se$_3$, and MoSe$_2$, the mechanisms which stabilize these structures can be understood. [2]

Compounds prepared from PbSe and VSe$_2$ layers show charge transfer between layers as well, allowing to tune transport properties via modulation doping. Additionally, the emergence of a charge density wave in the VSe$_2$ layers has been reported below 100 K [3], and was investigated by angle-resolved PES.

[1] Esters et al., *Angew. Chem. Int. Ed.* **54**, 1130 (2015).

[2] Göhler et al., *J. Phys. Chem. C* **125**, 9469 (2021).

[3] Cordova et al., *Chem. Mater.* **31**, 8473 (2019).

CPP 35.8 Thu 11:15 H17

Impact of opto-electronic measurements on the properties of hexagonal boron nitride as a dielectric — •Jo Bertram[1], Luca Kotewitz[1], Manfred Ersfeld[1], Frank Volmer[1], Kenji Watanabe[2], Takashi Taniguchi[3], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

Hexagonal boron nitride (hBN) serves as an atomically flat, insulating substrate for a large variety of 2D heterostructures. However, recent opto-electronic experiments showed that optically triggered leakage currents passing through hBN pose a serious bottleneck for reliable gating of 2D semiconductors [1]. Motivated by these observations, we report on photo-induced charge transport through hBN in graphite-hBN-graphite devices. Furthermore, we examine the impact of illuminating hBN employed as a gate dielectric on the charge carrier density of graphene Hall bar devices. Our results indicate that hBN exhibits optically active electronic states, which partially screen the gate electric field under light illumination. Interestingly, we observe a strong asymmetry of this effect for positive and negative electric fields showing that hBN does not behave as an ideal dielectric within the plate capacitor model especially in opto-electronic experiments.

[1] F. Volmer et al., Phys. Status Solidi RRL 14, 2000298 (2020)

CPP 36: Complex Fluids and Soft Matter 2 (joint session DY/CPP)

Time: Thursday 10:00–11:30 Location: H18

CPP 36.1 Thu 10:00 H18

Underscreening in the Restricted Primitive Model — •Andreas Härtel — Institute of Physics, University of Freiburg, Germany

Electric double layers occur where charges are screened by other charges, for instance, when charged surfaces of electrodes, colloids, or cells are exposed to electrolytes (mobile ions in a solvent). Increasing the concentration of mobile ions leads to more efficient screening, if concentrations are sufficiently low. At high concentrations, however, the screening by finite-sized ions becomes less efficient than those of point-like ions due to packing, an effect called underscreening. Some experiments report underscreening as a strong effect that follows some universal scaling [1], but the observation could not been explained by theoretical models yet. Conversely, independent theoretical studies actually ruled out the most important model for electrolytes of finite-sized ions as a candidate able to explain underscreening, namely the restricted primitive model [2]. In this talk I will discuss in which sense underscreening can and cannot be found in the restricted primitive model and in which sense the effect follows some universal scaling. I will support the discussion by recent theoretical results obtained from simulations and liquid state theories.

[1] Lee et al., Underscreening in concentrated electrolytes, Faraday Dicuss. 199, 239 (2017).

[2] Cats et al., Primitive Model Electrolytes in the Near and Far Field: Decay Lengths from DFT and Simulations, J. Chem. Phys. 154, 124504 (2021).

CPP 36.2 Thu 10:15 H18

Reciprocal and nonreciprocal eigenmodes of viscoelastic fluids — •Juliana Caspers[1], Clemens Bechinger[2], Nikolas Ditz[2], Matthias Fuchs[2], Felix Ginot[2], Karthika Krishna Kumar[2], Luis Frieder Reinalter[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August Universität Göttingen, 37073 Göttingen, Germany — [2]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Complex fluids such as wormlike micellar solutions are in general non-Markovian. In equilibrium, their behavior is often well approximated by a simple Maxwell model with one characteristic timescale [1]. Recoil experiments, after a colloidal probe has been sheared through the solvent, however, displayed a double-exponential relaxation [2]. We found excellent agreement of our measurements with a linear two-bath particle model. Depending on whether the optical trap which confines the probe is turned on or off, we find two sets of eigenmodes in our model, corresponding to either nonreciprocal (trap on) or reciprocal (trap off) forces. Using different recoil protocols as well as equilibrium mean square displacement measurements we confirmed the existence of these two different sets of timescales with experiments. Finally, for linear systems, we find a Volterra relation between two memory kernels, characterizing reciprocal and nonreciprocal forcing.

[1] F. Ginot, J. Caspers, M. Krüger, C. Bechinger. *Phys. Rev. Lett.* **128**, 028001 (2022)

[2] F. Ginot, J. Caspers, L. F. Reinalter, K. Krishna Kumar, M. Krüger, C. Bechinger. *arXiv:2204.02369* (2022)

CPP 36.3 Thu 10:30 H18

Elastic Turbulence in von Kármán geometry — •Reinier van Buel and Holger Stark — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Elastic turbulence, occurring in viscoelastic fluid flow at vanishing Reynolds numbers, is an interesting flow state [1-4] and has been experimentally studied in the von Kármán geometry [1]. Elastic turbulence is especially appealing for the mixing of fluids on the micron scale, which is extremely challenging in Newtonian fluids where transport relies on diffusion. Here, we present a fully three-dimensional numerical investigation of the von Kármán flow using the Oldroy-B model [4]. We observe a non-axisymmetric mode with four-fold symmetry that drives the flow instability towards elastic turbulence and compare it to results obtained from a linear stability analysis. By analyzing the velocity fluctuations and defining an order parameter, we identify a bistable flow state above a sub-critical transition, which switches between a weakly chaotic flow state and elastic turbulence and exhibits hysteretic behavior. Furthermore, we reveal a sharp increase in the flow resistance at the transition to elastic turbulence, which we attribute to the elastic contribution of the work performed at the open side surface of the flow. Finally, an analysis of the spatial and temporal velocity power spectra confirms the turbulent nature of the flow.

[1] A. Groisman and V. Steinberg, Nature **405**, 53 (2000).
[2] R. Buel, C. Schaaf, H. Stark, Europhys. Lett. **124**, 14001 (2018).
[3] R. Buel and H. Stark, Sci. Rep. **10**, 1-9 (2020).
[4] R. Buel and H. Stark, Phys. Fluids **34**, 4 (2022).

CPP 36.4 Thu 10:45 H18

Coarsening dynamics of quasi 2D emulsions in free-standing smectic films — •Christoph Klopp, Torsten Trittel, and Ralf Stannarius — Institute for Physics, Otto von Guericke University Magdeburg, Germany

Hydrodynamic phenomena in thin films play a crucial role in biological systems, in nature and modern technology. Various experimental and theoretical studies explored, e.g., the motion of objects in quasi two-dimensional films [1], the merging of inclusions [2-4] and the structural change of emulsions during long-term observations. Here, we demonstrate and describe the coarsening dynamics of emulsions formed by smectic islands (flat circular regions) on liquid crystal bubbles in microgravity at the International Space Station (ISS). The smectic islands form polydisperse, disordered arrangements representing quasi 2D emulsions. We analyze the time evolution of these ensembles that proceed through direct island coalescence or the exchange of material through the background film (Ostwald ripening). Coarsening is ubiquitous in liquid emulsions and foams, and important for their stability. We compare our results with such systems and analyze the dominant process for the 2D coarsening dynamics.

Acknowledgements: This study was supported by NASA, DFG and DLR within the OASIS and OASIS-Co projects.

References: [1] A. Eremin et al., Phys. Rev. Lett., 107, 268301 (2011) [2] N. S. Shuravin et al., Phys. Rev. E, 99, 062702 (2019) [3] Z. H. Nguyen et al., Phys. Rev. Research, 3, 033143 (2021) [4] C. Klopp et al., Soft Matter 16 4607 (2020)

CPP 36.5 Thu 11:00 H18

Phase transitions in the generalised chiral Lebwohl-Lasher model — •Philipp Elsässer and Anja Kuhnhold — Institute of Physics, Albert-Ludwigs-University Freiburg, Germany

The behaviour of liquid crystals can be described by using the Lebwohl-Lasher (LL) model, where unit vectors that resemble nematic directors are positioned on a simple cubic lattice. Due to the interaction potential, which favours parallel orientations, this model is well suited to analyse isotropic-nematic (IN) phase transitions.

There exist several extensions to this model with which its applicability can get further enhanced. We use two combined extensions to obtain the generalised chiral Lebwohl-Lasher model: We apply a generalisation to tune the sharpness of the potential, as in the work of Fish and Vink [1] and add a chiral term which is based on the work of Memmer et al. [2]. In this system we study the phase transition properties with the help of Monte Carlo simulations. To identify characteristic properties of the transitions, we apply finite-size scaling. This allows us to determine chirality-sharpness parameter pairs with which we can manipulate the nature of the transition between ordered and disordered states [3].

[1] J. M. Fish, R. L. C. Vink, PRE **81**, 021705 (2010).
[2] R. Memmer, O. Fliegans, PCCP **5**, 558 (2003).
[3] P. Elsässer, A. Kuhnhold, PRE **105**, 054704 (2022).

CPP 36.6 Thu 11:15 H18

Systematic parametrization of non-Markovian dissipative thermostats for coarse-grained molecular simulations with accurate dynamics — •Viktor Klippenstein and Nico F. A. Van Der Vegt — Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Technische Universität Darmstadt, 64287 Darmstadt, Germany

The Mori-Zwanzig theory, in principle, allows to derive an exact equation of motion for coarse-grained degrees of freedom based on the dynamics of an underlying fine-grained reference system.[1] Still, in practice the simultaneous representation of structural and dynamic properties in particle-based models poses a complicated problem, e.g. due to the non-linearity of the exact coarse-grained equation of motion.

A viable approximate approach is to start from a conservative coarse-grained force-field and to extend the standard Newtonian equation of motion used in molecular simulation with a linear generalized Langevin thermostat. We demonstrate how such a thermostat can be parametrized to correctly represent dynamic properties, both in a purely bottom-up approach[2,3] or by applying iterative optimization.[3] We consider the Asakura-Oosawa model as a test case.[3]

[1] V. Klippenstein, M. Tripathy, G. Jung, F. Schmid, and N. F. A. van der Vegt, The Journal of Physical Chemistry B 125, 4931 (2021).
[2] V. Klippenstein and N. F. A. van der Vegt, The Journal of Chemical Physics 154, 191102 (2021).
[3] V. Klippenstein and N. F. A. Van Der Vegt, The Journal of Chemical Physics under review (2022).

CPP 37: Interfaces and Thin Films and Responsive and Adaptive Systems

Time: Thursday 10:30–13:00 Location: H39

Invited Talk CPP 37.1 Thu 10:30 H39

Non-equilibrium Properties of Thin Polymer Films — •Günter Reiter[1] and Sivasurender Chandran[2] — [1]Physikalisches Institut, Albert-Ludwigs Universität Freiburg — [2]Department of Physics, Indian Institute of Technology Kanpur, Uttar Pradesh 208016, India

Rapid industrial processes often freeze polymers in non-equilibrium conformations, which, in turn, cause material properties that are significantly different from the predictions of equilibrium theories. Thus, by choosing appropriate processing pathways, we potentially can control macroscopic properties and performance of polymers. However, due to our current lack of fundamental understanding of the behavior of non-equilibrated polymers, we have to rely on empirical knowledge, imposing trial-and-error approaches for achieving desired properties. Considering these aspects, we discuss recent studies on polymer films revealing that quantitative relations exist between properties and processing pathways, suggesting possible relations for processing-induced deviations in chain conformations. These relations propose that long-living and long-ranged correlations between polymers have been induced by processing, as indicated by the observation of relaxation times much longer than known for equilibrated polymers. We present an example where control of processing conditions for thin films allowed to translate the molecular relaxations during equilibration into a predictable lifting of macroscopic loads.

CPP 37.2 Thu 11:00 H39

Water Induced Polymer Reorientation at a Polystyrene/Polyacrylic Acid Surface — Xiaomei Li[1], Mirela Encheva[2], Kaloian Koynov[1], Hans-Jürgen Butt[1], Ellen Backus[2], and •Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]University of Vienna, Währinger Straße 42, 1090 Vienna, Austria

Polymers are capable of undergoing adaptation phenomena triggered by exposure to liquids. Here we study the adaptation of copolymer films formed by polystyrene and polyacrylic acid (PS/PAA) after water exposure. We measured the dynamic advancing and receding contact angles (CA) of water drops sliding down a PS/PAA film. We associate the gradual increase in advancing CA with drop velocity to the adaptation process to water. By applying adaptation theory, we estimated the time constant of this adaptation process to be much smaller than 1 s. The changes in contact angles may be caused by swelling of the copolymer and/or by a reorientation of the hydrophilic segments (PAA) towards the surface. Therefore, we performed vibrational sum frequency generation (SFG) spectroscopy which is surface sensitive. SFG experiments before and after exposing the copolymer to water reveal a decrease in intensity of the vibrational band representing the PS segments, suggesting a reorientation of the polymer groups at the surface upon contact with water.

15 min. break

CPP 37.3 Thu 11:30 H39

Tailoring the Optical Properties of Sputter-Deposited Gold

Nanostructures on Nanostructured TiO2 Templates based on in situ GISAXS Determined Growth Laws — •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], Ya-Jun Cheng[5], and Peter Müller-Buschbaum[1,6] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]LS Materialverbunde, Institut für Materialwissenschaft, CAU, 24143 Kiel — [3]DESY, 22607 Hamburg — [4]Department of Fibre and Polymer Technology, KTH, SE-100 44 Stockholm, Sweden — [5]NIMTE, CAS, 315201 Ningbo, China — [6]MLZ, TU München, 85748 Garching

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, meanwhile in situ GISAXS during the deposition process is applied to in-depth understand the Au morphology on the TiO2 templates. 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 37.4 Thu 11:45 H39

Investigations of ultra-thin film behavior of polycarbonate on inorganic surfaces — •Hassan Omar, Paulina Szymoniak, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Thin polymer films are of vital importance due to their low production costs and wide range of applications in sensors, electronics, and coatings. Their geometry is ideal for the study of confinement effects on the thermodynamic properties and segmental dynamics of polymers. However, there is little research into these effects for main chain polymers such as polycarbonate (PC). PC has important applications due to its improved mechanical, optical, and thermal stability compared to other polymers. For this investigation, films of PC ranging from 200 nm to 7 nm were prepared on both glass and silica substrates to measure the dielectric and calorimetric behavior. The methodology consisted of broadband dielectric spectroscopy (BDS), ellipsometry, atomic force microscopy (AFM), and sum frequency generation (SFG). Using ellipsometry, the glass transition was shown to increase with decreasing film thickness. This was further proved by BDS for glassy dynamics for thin films employing different sample geometries (crossed electrode and nanostructured capacitors). The properties and influence of the adsorbed layer on the molecular mobility was also addressed by a combination of AFM, SFG and BDS.

CPP 37.5 Thu 12:00 H39

Fabrication and Characterization of Hydrophobic Porous Metallic Membranes for High-Temperature Applications — Sara Claramunt[1], •Muhammad Khurram[2], Walther Benzinger[1], Manfred Kraut[1], and Roland Dittmeyer[1] — [1]Institute for Micro Process Engineering, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Physics, University of Greifswald, 17489 Greifswald, Germany

Hydrophobic porous metallic membranes can be integrated into a microreactor for in-situ separation of steam at high temperatures. This study investigates the fabrication and characterization of hydrophobic coatings on metallic substrates. Two different coating methods were explored: (1) plasma enhanced-chemical vapor deposition to form amorphous carbon silicon-doped a-C:H:Si:O thin films and (2) direct immersion in fluoroalkyl silane (FAS-13) solution using dip coating to form self-assembled monolayers. The results on wettability as well as SEM images and Energy Dispersive Spectroscopy/Wavelength Depressive Spectroscopy analyses indicate that the coated sintered stainless-steel membranes are adequate as hydrophobic surfaces, maintaining the porosity of the substrate and withstanding high temperatures. Especially the FAS-13 coating shows very good resistance to temperatures higher than 250°C. These findings are of special significance for the fabrication of porous metal membranes for the separation of steam in high-temperature applications.

CPP 37.6 Thu 12:15 H39

Superlatice deformation via uniaxial strain and its impact on photoluminescence in PbS quantum dot thin films — •Julian E. Heger[1], Wei Chen[1], Huaying Zhong[1], Tianxiao Xiao[1], Constantin Harder[1,2], Fabian A. C. Apfelbeck[1], Alexander Weinzierl[1], Regine Boldt[3], Lucas Schraa[3], Eric Euchler[3], Anna K. Sambale[3], Konrad Schneider[3], Matthias Schwartzkopf[2], Stephan V. Roth[2,4], and Peter Müller-Buschbaum[1,5] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]Leibniz-Institut für Polymerforschung IPFDD, 01069 Dresden — [4]Royal Institute of Technology KTH, 100 44 Stockholm — [5]MLZ, TU München, 85748 Garching

Colloidal lead sulfide quantum dots (PbS CQDs) show high potential for the application in flexible electronics, as they are solution processible with tunable optoelectronic properties. In thin films, PbS CQDs form a superlattice morphology that tailors these optoelectronic properties. For instance, electronic coupling between adjacent PbS CQDs is dependent on the inter-dot distance in the superlattice. In this work, we investigate the superlattice deformation during applied external strain. For this, PbS CQDs thin films are prepared on flexible PDMS substrates. The samples are investigated with in situ GISAXS and photoluminescence measurements at different levels of strain to correlate the deformation-induced morphological changes to the optoelectronic performance.

CPP 37.7 Thu 12:30 H39

The surface of electrolyte solutions is stratified — •Yair Litman, Kuo-Yang Chiang, Takakazu Seki, Yuki Nagata, and Mischa Bonn — MPI for Polymer Research, Mainz, Germany.

The electrical-double layer (EDL) model has been used during the last two decades to describe the behaviour of ions at the water/air interface, and also as a framework to analyze and interpret several types of surface-selective experimental measurements. In this work, we present a combination of surface-sensitive heterodyne-detected vibrational sum frequency generation (VSFG) and *ab initio* based molecular dynamics simulations to study the liquid/air interface of different aqueous electrolyte solutions. Our VSFG measurements clearly demonstrate that the EDL model is an incomplete microscopic picture to understand the interface of NaCl, NaBr and NaCl aqueous solutions and it is completely inappropriate for the NaOH and CsF cases. Based on our simulations, we propose that the surface of electrolytes solutions is stratified into two water layers, one depleted and the other enriched with ions, creating an effective liquid-liquid interface buried a few Å inside the solution.

CPP 37.8 Thu 12:45 H39

A purely ionic voltage effect soft triod — •Elalyaa Mohamed, Sabine Josten, and Frank Marlow — Kaiser-Wilhelm-Platz 1, 45470 Mülheim an der Ruhr

Iontronics is a concept of connecting ionic transport, storage and reactions with electronics. As ions are the language of nature and electrons are the language of man-made information processing, connecting both may lead to more understanding of nature as well as to new computational systems which might be called neuromorphic. In the last decade, many iontronic devices were invented and studied. However, developing of iontronics requires the invention of more flexible devices. In our lab we developed a purely ionic voltage effect soft triode (IVEST) based on interfacial ion adsorption and redox oxidizer depletion. The IVEST was built with no need of sophisticated or expensive materials. This device is an electrochemical micro-cell, which consists of a top electrode and two bottom electrodes. The basic idea of this device is to control the concentration and diffusion of ions by the voltage applied on the top electrode. In different electrical circuit configurations, it can show amplification or memory effects. The device had an electrical current amplification reaching 52 and memory effects in the electrical resistance lasting for up to 6 h. These values were achieved by tuning an electrode interface, the electrolyte and diffusion properties. They might be promising for neuromorphic applications.

CPP 38: 2D Materials 9 (joint session HL/CPP/DS)

Time: Thursday 11:15–12:15 Location: H36

CPP 38.1 Thu 11:15 H36

Generating extreme electric fields in 1 2D materials by dual ionic gating — •Benjamin Isaac Weintrub[1], Yu-Ling Hsieh[1,2], Jan N. Kirchhof[1], and Kirill I. Bolotin[1] — [1]Department of Physics, Freie Universität Berlin, Berlin, Germany — [2]Department of Mechanical Engineering, National Central University, Taoyuan City, Taiwan

We demonstrate a new type of dual gate transistor to induce record electric fields through two-dimensional materials (2DMs). At the heart of this device is a 2DM suspended between two volumes of ionic liquid (IL) with independently controlled potentials. The potential difference between the ILs falls across an ultrathin layer consisting of the 2DM and the electrical double layers above and below it, thereby producing an intense electric field across the 2DM. We determine the field strength via i) electrical transport measurements and ii) direct measurements of electrochemical potentials of the ILs using semiconducting 2DM, WSe2. The field strength across a bilayer WSe2 sample reaches ~2.5 V/nm, the largest static electric field through the bulk of any electronic device to date. Additionally, we create electric fields strong enough to close the bandgap of 3-layer and 4-layer WSe2 (~1.4 V/nm and ~0.9 V/nm respectively). Our approach grants access to previously-inaccessible phenomena occurring in ultrastrong electric fields.

CPP 38.2 Thu 11:30 H36

Tip-enhanced Raman spectroscopy combined with other Scanning Probe Microscopy Methods: Focus on 2D Materials — •Jana Kalbacova — HORIBA Jobin Yvon GmbH, Neuhofstr. 9, Bensheim 64625, Germany

New two dimensional materials are on the rise. After the wonder material graphene, new materials such as MoS2, MoSe2, WSe2 have an intrinsic bandgap and as such are opening new doors for semiconductor applications. Raman spectroscopy offers information on the chemical structure of materials but cannot provide information on the electronic properties such as surface potential or photocurrent of our sample. Co-localized measurements combining scanning probe microscopy (SPM) with Raman spectroscopy can already bring a wealth of information; however, further improvements can be obtained by a tip that will act as an antenna and amplify the Raman signal and thus breaking the diffraction limit in a method called Tip-enhanced Raman spectroscopy (TERS). Typically spatial resolution of 10 - 20 nm can be achieved. In this contribution, we investigate different 2D materials by a combination of TERS, tip-enhanced photoluminescence, Kelvin probe microscopy, and other SPM methods to show very locally for example doping variations or defects that would otherwise go unnoticed with other macro- and microscopic techniques.

CPP 38.3 Thu 11:45 H36

Defects in 2D WS_2 monolayers — Aswin Asaithambi[1], Roland Kozubek[1], Francesco Reale[2], Erik Pollmann[1], Marcel Zöllner[1], Cecilia Mattevi[2], Marika Schleberger[1], Axel Lorke[1], and •Günther Prinz[1] — [1]Fakultät für Physik und CENIDE, Universität Duisburg-Essen, Germany — [2]Department of Materials, Imperial College London, UK

In this presentation, we report about optical characterization and manipulation of defects in tungsten disulfide (WS_2) monolayers. WS_2 is one prominent member of the 2D transition metal dichalcogenides (TMDC). In these materials, defects and adsorbates can easily modify e.g., conductivity, optical properties, or even create single photon emitters. For this study we used high quality WS_2 CVD-grown monolayers to purposely introduce defects via irradiating them with Xe^{30+} ions with different fluences [1]. Low temperature photoluminescence (PL) spectra of these irradiated WS_2 monolayers show two defect related broad bands, beside the excitonic contribution. By exposing these flakes to laser light with powers up to 1.5mW, the intensity of these two PL bands can be reduced. By comparing the intensity of the excitonic contribution before and after this laser processing, we don't observe an increase in intensity, leading us to conclude, that the defects aren't getting healed. If the samples are heated to room temperature, the defect luminescence recovers. To interpret our observation, we suggest that the defects might be attributed to vacancy defects together with adsorbates at different defect sites.

[1] A. Asaithambi et al., Phys. Status Solidi RRL 2021, 15, 2000466

CPP 38.4 Thu 12:00 H36

Large perpendicular field in bilayer TMD via hybrid molecular gating — •Sviatoslav Kovalchuk[1], Abhijeet Kumar[1], Simon Pessel[1], Kyrylo Greben[1], Dominik Christiansen[2], Malte Selig[2], Andreas Knorr[2], and Kirill Bolotin[1] — [1]Department of Physics, Quantum Nanoelectronics of 2D Materials, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We consider structures in which bilayer TMDs are sandwiched between a layer of molecules and Si gate. We show that these structure allow increasing, by a factor of 2, maximum electric field achievable in this 2D material. This in turn, allows reaching electric field >0.2 V/nm. In MOS2 this is sufficient to bring interlayer excitons IX into resonance with either A or B intralayer excitons. We study coupling between these excitons, and give an outlook on the new technique to achieve large perpendicular electric fields detectable in optical measurements.

CPP 39: Molecular Electronics and Excited State Properties

Time: Thursday 11:30–13:00 Location: H38

CPP 39.1 Thu 11:30 H38

Fluorinated Acenes: Controlling Molecular Electronic Levels, Crystalline Phases and Optoelectronic Properties — •Daniel Bischof[1], Philipp E. Hofmann[2], Matthias W. Tripp[2], Marc Zeplichal[3], Sebastian Anhäuser[1], Tobias Breuer[1], Sergei I. Ivlev[2], Marina Gerhard[1], Andreas Terfort[3], Ulrich Koert[2], and Gregor Witte[1] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]Fachbereich Chemie, Philipps-Universität Marburg — [3]Goethe Universität Frankfurt

Acenes serve as prototypical molecular materials to study structure-property relationships. Here, we systematically analyze the influence of the acene length and the degree of fluorination on their structure and optoelectronic properties [1-3]. Our results show that the optical gap decreases with increasing acene length, while the degree of fluorination determines the precise energy levels of the frontier orbitals HOMO and LUMO, whereas the optical gap is barely affected upon fluorination. Partial fluorination also influences the molecular electrostatic potential (MEP) and leads to a change in the molecular packing from herringbone packing for pristine and perfluorinated acenes to a planar stacking motif. These structural changes also affect the photoluminescence properties and induce a red-shifted PL for the stacked molecules due to excimer formation. The presented insights are not limited to acenes, but can be extended to other π-conjugated systems.

[1] P. E. Hofmann, et al. Angew. Chem. Int. Ed. 59, 16501 (2020).
[2] D. Bischof et al. J. Phys. Chem. C 125, 19000 (2021).
[3] D. Bischof et al. Chem. Eur. J. 28, e202103653 (2022).

CPP 39.2 Thu 11:45 H38

Time-resolved spectroscopy study of the dynamics of charge transfer processes in strongly interacting organic donor/acceptor compounds — •Nico Hofeditz[1], Christoph P. Theurer[2], Julian Hausch[2], Katharina Broch[2], Wolfram Heimbrodt[1], and Marina Gerhard[1] — [1]Department of Physics, Philipps-Universität Marburg, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Germany

Doping of organic semiconductors with strong acceptor molecules is an effective way to tailor their electronic properties. Here, we investigate the photoexcitation dynamics of blends of tetracene and the strong acceptor F4-TCNQ to better understand how acceptors alter the transport of charge carriers and excitons. The mixtures feature a phase of relatively pure tetracene as well as an intimately mixed phase. In the mixed phase donor and acceptor molecules for charge transfer complexes that efficiently quench excitons from the pure phases. That leads to faster photoluminescence dynamics in the blends with respect to neat tetracene. We investigate the low temperature photoluminescence through global analysis and find constrained dynamics in the blends which we attribute to localization effects and energetic disorder in the tetracene domains.

CPP 39.3 Thu 12:00 H38

Ultrafast excited states dynamics of two orthogonal molecular photoswitches — •Tanja Schmitt[1], Li-Yun Hsu[2], Eva Blasco[2], and Petra Tegeder[1] — [1]Physical Chemistry, Ruprecht-Karls-Universität Heidelberg — [2]Organic Chemistry, Ruprecht-Karls-Universität Heidelberg

Molecular photoswitches are widely used in physics, chemistry, biology and material sciences. The use of multiple photoswitches at one time opens diverse opportunities for further improved and more complicated systems. This requires orthogonal addressability of the photoswitches and ideally reversible processes. Herein, we report a mixture of two reversible and orthogonal photoswitches which could potentially be used in four-dimensional printing. We report the first study of their ultrafast excited state dynamics when they are addressed orthogonally as well as simultaneously to gain insight in their interaction. In addition, the environmental influence of the excited state dynamics of the orthogonal photoswitches is examined using different solvents as well as films.

CPP 39.4 Thu 12:15 H38

Charge Transfer and Singlet Fission in Pentacene/Acceptor thin films — •Martin Richter[1], Christoph Theurer[2], Debkumar Rana[1,3], Katharina Broch[2], and Petra Tegeder[1,3] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 253/229, 69120 Heidelberg, Germany — [2]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [3]Centre for Advanced Materials, Universität Heidelberg, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany

Singlet fission (SF) is a process where a singlet excited state is converted into two triplet excited states. Since SF is exothermic in pentacene (PEN), it is an excellent material to investigate charge transfer (CT) interactions with electron acceptors. Here, stacked bi-layers of PEN either with 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) or 2,2'-(perfluoronaphthalene-2,6-diylidene)dimalononitrile (F6-TCNNQ) were investigated with transient absorption spectroscopy. The experiments show formation of triplet pairs, due to the SF process with a slightly slower time constant compared to the pure PEN. Subsequently a separation of the correlated triplet pair can be observed, a process that has been identified also in PEN thin films. A drastic reduction of the triplet lifetime is extracted with both acceptors. Further, evidence for diffusion of excitons to the interface followed by charge formation is found for layers with F4-TCNQ, supported by the shifting of an absorption band, caused by electric fields.

CPP 39.5 Thu 12:30 H38

Understanding charge transfer excitations in Bacteriochlorophyll dimers from first principles — •Zohreh Hashemi[1], Matthias Knodt[1], and Linn Leppert[1,2] — [1]Institute of Physics, University of Bayreuth, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Netherlands

Bacteriochlorophyll (BCL) molecules are the main pigments driving the primary excitation and charge transfer processes in photosynthetic bacteria. They are organized in highly coordinated multichromophoric complexes, embedded in protein, guaranteeing an efficient transfer of excitation energy from the light harvesting antennae to the reaction center where a charge transfer excitation triggers. In this contribution we focus on the electronic and excited state structure of BCL monomers and dimers found in the reaction center and light harvesting apparatus of the purple bacterium Rhodobacter sphaeroides. We asses the accuracy of ab initio GW+Bethe-Salpeter equation approach for BCL monomers considering a wide range of excitation energies, and find excellent agreement with experimental data and correlated wavefunction-based approaches. We also discuss notable differences to results from state-of-the-art time-dependent density functional theory, which can be traced back to the treatment of electron-hole interactions in both methods [1]. For dimeric systems we show that the energy and character of charge transfer excitations is strongly affected by distance and orientation of the BCL molecules, providing an intuitive understanding for the role of these excitations in different parts of the photosynthetic apparatus.

CPP 39.6 Thu 12:45 H38

Temperature Dependent Optical Transition in Zinc Phthalocyanine Single Crystals — •Lisa Schraut-May[1], Sebastian Hammer[1], Kilian Frank[2], Bert Nickel[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]Department of Physics and Center for Nano Science, Ludwig Maximilian University, 80539 Munich — [3]Bavarian Center for Applied Energy Research, 97074 Würzburg

By its various polymorphs, Zinc Phthalocyanine (ZnPc) serves as an excellent model system to study the interplay between molecular packing on microscopic length scales and the resulting photophysical properties [1]. Here, we address the dependence of the excitonic coupling on the underlying crystal structure of the thermodynamically stable ZnPc β-phase. For this purpose, we conducted complementary temperature dependent X-ray diffraction as well as polarisation dependent photoluminescence (PL) studies on ZnPc single crystals. By means of the PL signals spectral characteristics we observed a continuous transition from a J- into an H-aggregated state between 300 K and 100 K. Remarkably, below 100 K an exceptionally sharp PL peak evolves being indicative for the formation of a superradiant J-aggregate. As there is no indication for a discrete structural phase transition, we interpret the resulting PL signal in this temperature range by a model of vibronically coupled excitons steered by the gradual anisotropic thermal contraction of the crystal lattice [2]. We thank the Bavarian research network SolTech for financial support. [1] Hammer et al., Appl. Phys. Lett. (2019) [2] Hestand et al., Chem. Rev. (2018)

CPP 40: Organic Electronics and Photovoltaics 3

Time: Thursday 15:00–17:45 Location: H38

Invited Talk CPP 40.1 Thu 15:00 H38

Computational Design of Organic Semiconductors — •Harald Oberhofer — Chair for Theoretical Physics VII, Universität Bayreuth — Chair for Theoretical Chemistry, Technische Universität München

Organic electronics—in the form of field effect transistors, light emitting diodes, or solar cells—are slowly finding their use in everyday consumer devices. To date, most of the employed materials have been discovered by structural tuning of a promising compound family, thereby relying on intuition, experience, or simply trial and error. While sometimes quite successful, such incremental changes only lead to a local exploration of the vast chemical space of possible molecules, potentially overlooking many interesting materials.

In contrast, modern data-driven strategies allow the extraction of general design rules through the systematic of the available design space. Often, these take the form of a computational funnel, where large databases are searched by computing relevant properties, so-called descriptors, for each element of the database. While this can point towards promising yet so-far overlooked theoretical and experimental design routes for organic electronics materials such an approach is limited by the employed database, not really allowing any insight beyond. Therefore, we trained machine-learned surrogate models for the most important organic semiconductor properties. These form the basis for an active machine learning scheme that allows us to sample the, in principle, unlimited space of organic molecules searching for materials not considered so far.

CPP 40.2 Thu 15:30 H38

Reorganization energies of flexible organic molecules as

a challenging target for machine learning enhanced virtual screening — •Ke Chen[1,2], Christian Kunkel[1,2], Karsten Reuter[1,2], and Johannes T. Margraf[1,2] — [1]Technische Universität München, Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The molecular reorganization energy λ strongly influences the charge carrier mobility of organic semiconductors and is therefore an important target for molecular design. Machine learning (ML) has the potential to accelerate this process by providing accurate surrogate models in design space. Unfortunately, λ poses a significant challenge for ML-models as it simultaneously depends on the neutral and ionized potential energy surfaces of the molecule.

In this contribution, we address the questions of how ML models for λ can be improved and what their benefit is in high-throughput virtual screening (HTVS). We find that, while improved predictive accuracy with respect to a semi-empirical baseline model is achieved, the benefits for molecular discovery are actually somewhat marginal. In particular, ML-enhanced HTVS is more effective in identifying promising candidates but leads to a less diverse sample set.

CPP 40.3 Thu 15:45 H38

Protonation-Induced Charge Transfer and Polaron Formation in Organic Semiconductors Doped by Lewis Acids — •Fabian Bauch, Chuan-Ding Dong, and Stefan Schumacher — Physics Department and CeOPP, Paderborn University, Germany

Organic electronics rely crucially on doping to enhance the conductivity of organic semiconductors (OSC). Lewis acid doping of OSC is currently of great interest as an alternative to typical molecular p-type doping. Recently, the underlying process was understood to be based on the electron transfer (ET) from a neutral polymer to the protonated polymer [Nat. Mater. 18, 1327 (2019)]. In this work, we provide insight into the microscopic process by investigating the influence of protons on the electronic properties of the copolymer PCPDT-BT using DFT calculations. [1] We find that a single proton on the backbone can give rise to a polaron coupled to the proton position. Two protons on the same polymer backbone can induce a long range intrachain ET, resulting in a polaron decoupled from the proton positions, more fit to act as charge carrier. We also demonstrate the possibility of ET between a neutral polymer and a doubly protonated polymer. The experimental data on the doping of PCPDT-BT via Lewis acid BCF agree well with our simulated vertical excitation spectra for an ensemble of protonated species with increasing amounts of protons. Our results highlight the important role of multiple protonation of the OSC backbone in completing the mechanistic picture of Lewis acid doping. [1] F. Bauch, C. Dong, and S. Schumacher, RSC Advances 12, 13999 (2022).

CPP 40.4 Thu 16:00 H38

Adsorption layers of diketopyrrolopyrrole acceptor blocks on graphite: Self-assembly and structure in all-atom modelling — Moufdi Hadjab[1] and •Olga Guskova[2] — [1]Boudiaf University of M'Sila, 28000 M'Sila, Algeria — [2]IPF Dresden, 01069 Dresden, Germany

In this computational work, we investigate the adsorption layers of electron-deficient N-unsubstituted difuran-diketopyrrolopyrroles (DPP). Three conformational states differing in the mutual orientation of the central DPP unit and furan flanks are distinguished: cis-cis, trans-trans, and cis-trans. The adsorption layers are obtained during in-silico self-assembly on graphite surface through intermolecular hydrogen bonding in all-atom MD simulations. The experimental process for the construction of the adsorption layers, called the droplet deposition technique, is reproduced in the modeling. In all simulated systems, the formation of stable supramolecular polymers is observed which build the ordered carpets on the surface. However, the binding energetics and strength and the type of hydrogen bonding are highly sensitive to the molecular conformation. We quantify each of these characteristics and provide a molecular picture of difuran-DPP layers relevant for organic field-effect transistor applications. OG thanks DFG (project GU1510/5-1) for financial support.

CPP 40.5 Thu 16:15 H38

Understanding Phonon Properties and the Thermal Conductivity of Crystalline Polymers — •Lukas Reicht, Lukas Legenstein, Tomas Kamencek, Sandro Wieser, and Egbert Zojer — Graz University of Technology, Austria

Disordered polymers are characterized by a very low thermal conductivity on the order of 0.1 W/mK. In contrast, recent studies have shown that aligned (crystalline) polymers can have thermal conductivities comparable to those of metals. Given these prospects, it is interesting to understand, how the thermal conductivity of a polymer depends on its chemical structure. A crucial step in that context is to investigate phonons and their influence on thermal transport. For simulating the phonons, we relied on density-functional theory (DFT) calculations combining phonopy and the Vienna Ab initio Simulation Package (VASP). In a second step, anharmonic force constants and thermal conductivities were calculated with phono3py and hiPhive. Additionally, we explored the capabilities of on-the-fly machine learned force fields (ML-FF), trained on DFT data, as implemented in VASP. These approaches were tested and benchmarked for polyethylene as a comparably simple model system. The final goal of our work is to then apply the above methodology to other polymers, systematically varying the structure of the backbone, thereby finding structure-to-property relations. These polymers include poly(p-phenylene), polythiophene, polyfuran, polyselenophene, poly(3-hexylthiophen-2,5-diyl) (P3HT) and Poly(p-phenylene vinylene) (PPV).

15 min. break

CPP 40.6 Thu 16:45 H38

Assessing Crystal Structure Prediction Based on Density Functional Tight Binding and Evolutionary Algorithms — •Sebastian Hutsch and Frank Ortmann — Department of Chemistry, Technical University of Munich

The prediction of crystal structures for organic molecules is a computationally expensive task due to the large number of atoms in the unit cell and the associated number of possible configurations. The computational load can be compensated by the use of classical force fields, which however lack transferability to new molecules and necessitate an extensive training for complex molecules. Here, we study an approach to crystal structure prediction based on evolutionary algorithms and a combination of Density Functional Tight Binding (DFTB) and Density Functional Theory (DFT). This combination allows us to efficiently compute crystal structures for new materials on a high level of accuracy. A comparison of the calculated crystal structures with experimentally known structures will be made.

CPP 40.7 Thu 17:00 H38

Singlet Fission search in polyacene molecules in gas-phase and on rare-gas clusters using ab initio methods — •Selmane Ferchane[1], Alexander Eisfeld[2], and Michael Walter[1,3,4] — [1]Institute of Physics, University of Freiburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]FIT Freiburg Center for Interactive Materials and Bioinspired Technologies, University of Freiburg, Germany — [4]Fraunhofer IWM, Freiburg, Germany

Singlet fission (SF), is a spontaneous photo-excited splitting phenomenon. Where an organic chromophore dimer, converts its singlet exciton into a pair of triplet excitons. A great promise for future photon-to-current conversion of solar energy using organic materials with high efficiency. To get more insight into these processes of SF, we employed different ab initio theories and approaches in our investigation, namely, density functional theory (DFT), TD-DFT, MCTDH, and CASPT2/CASSCF. Since the spatial orientation is crucial to whether the molecule will go SF and the rate of it due to the orbital coupling of both molecules, based on recent studies. We calculate the most favorable orientation of the chromophores with the binding energies in the gas phase and adsorbed on Argon and Neon surfaces. Then we calculate the lowest-lying excited states that contribute to the singlet and triple transition plus the search for the possible conical intersection that crosses the surface potential energies.

CPP 40.8 Thu 17:15 H38

Materials design based on theoretical characterization: Improving open-shell organic molecules for electronic applications — •Sebastian Schellhammer[1] and Frank Ortmann[2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, 01187 Germany — [2]Department of Chemistry, Technische Universität München, Lichtenbergstr. 4, 85748 Garching b. München

In recent years, organic molecules with stable open-shell ground states have attracted growing interest due to their outstanding properties, i.e. responsive spin structures, high-spin ground states, two-photon absorption, or small band gap. Although a growing number of interesting materials has appeared, molecules often lack thermal stability impeding their application in electronic devices. In this presentation, we will highlight routes but also dead ends in the quest for high-spin configurations in hydrocarbons. We benchmark a computational approach for the characterization of open-shell organic structures, which combines predictability with appropriate simulation resources. For polycyclic heteroaromatic hydrocarbons containing a benzoisoindole core, we explain why a supposedly open-shell material does not provide the desired characteristics. On the contrary, we discuss the promising characteristics of stable polycyclic hydrocarbon diradicaloids as well as related tetraradicaloids. Based on these analyses, design rules for optimized material properties are extracted, which helps to exploit the full potential of promising material groups.

CPP 40.9 Thu 17:30 H38

Simulation organic semiconductors with tensor network techniques — •Sam Mardazad[1], Yihe Xu[2], Xuexiao Xang[2], Martin Grundner[3], Ulrich Schollwöck[3], Haibo Ma[2], and Sebastian Paeckel[3] — [1]Heriot-Watt University, Edinburgh — [2]School of Chemistry and Chemical Engineering, Nanjing University — [3]Department of Physics, Arnold Sommerfeld Center of Theoretical Physics, University of Munich

Organic solar cells provide the possibility to enhance the efficiency and to overcome the Shockley-Queisser limit. In this talk we present results for the simulation of quantum transport effects in a tetracene para dimers, a large organic molecule modelled by a Frenkel-exciton Hamiltonian. We account for the full quantum dynamics going beyond the Born-Oppenheimer approximation. For that purpose we use a new numerically unbiased representation of the molecule's wave function enabling us to compare with experiments, exhibiting good agreement. With this powerful approach we map out a phase diagram aiming and determining the experimental sweet spot yielding the highest charge carrier production rate. Furthermore, we develop a physical picture indicating that the coherent time scale in which most of the yield is generated is driven by a renormalization of the bare modes and make suggestions on how to manipulate this for the development of more efficient organic solar cells.

CPP 41: Crystallization, Nucleation and Self-Assembly

Time: Thursday 15:00–17:30 Location: H39

Invited Talk CPP 41.1 Thu 15:00 H39

Interface-induced crystallization in polymers: From model systems to applications for semiconducting polymers — Muhammad Tariq[1], Robert Kahl[1], Mukundan Thelakkat[2], Thomas Thurn-Albrecht[1], and •Oleksandr Dolynchuk[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg — [2]Applied Functional Polymers, University of Bayreuth

Crystallization is usually initiated at interfaces. Understanding the physical process underlying interface-induced crystallization (IIC) is of fundamental interest and is relevant for material applications. IIC of liquids can occur either by heterogeneous nucleation (HN) or by the equilibrium phenomenon of prefreezing. First, we present a combined theoretical and experimental study of the effect of the substrate-material interactions on the thermodynamics of prefreezing and on the kinetics of HN in model polymers on various substrates. Second, the acquired knowledge about IIC elucidates the role of interfaces for crystal orientation in films of conjugated polymers, which is important for device performance. Using polythiophenes as model conjugated polymers, we show that different crystal orientations can be formed at the interfaces to a substrate and vacuum as a result of two competing interfacial interactions. Our results demonstrate that increasing the polarity of polythiophene side chains influences the interactions at the interfaces, resulting in a change of crystal orientations. Thus, we disclose the crucial role of the interfacial interactions for crystallization kinetics, thin film morphology, and control of molecular orientation in films of model and semiconducting polymers.

CPP 41.2 Thu 15:30 H39

Determination of Morphologically Tailored Chirality in Supramolecular Nanostructures by X-ray Scattering — •Asena Cerhan Haink[1], Felix Wenzel[2], Klaus Kreger[2], Hans-Werner Schmidt[2], Richard Hildner[3], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung-Herzig Group, Universität Bayreuth,Universitätsstr.30, 95447 Bayreuth,Germany — [2]Makromolekulare Chemie I,Universität Bayreuth, Universitätsstr.30, 95447 Bayreuth,Germany — [3]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, Netherlands

Designed supramolecular nanostructures allow control over their optical and electronic properties which make them promising candidates for light-harvesting applications. Recently, we presented long-range (μm) transport of excitation energy in supramolecular nanofibres based on a carbonyl-bridged triarylamine (CBT). Here, we study supramolecular CBT building blocks with chiral side groups, which result in a distinct circular dichroism (CD) signal from self-assembled nanofibres. For bundles of supramolecular nanofibres, we observe an inversion in the CD signal as a function of temperature. To understand the origin of this effect, we performed morphological characterisation using temperature-dependent Wide Angle X-ray Scattering on the CBT-based bundles. We demonstrate systematic temperature-dependent variations in the π-π stacking and the column-column distances, which indicates that the CBT-based bundles have thermoelastic behaviour and change chirality at the critical temperature.

CPP 41.3 Thu 15:45 H39

Learning the Crystallisation Behaviour of Bidisperse Branched Model Polymers using Coarse-Grained Molecular Dynamics Simulations — •William Fall[1], Joerg Baschnagel[1], Olivier Lhost[2], and Hendrik Meyer[1] — [1]Institut Charles Sadron, 23 rue du Loess, 67034 Strasbourg Cedex, France. — [2]TotalEnergies One Tech Belgium, Zone Industrielle C, 7181 Feluy, Belgium

Model polymer systems allow fundamental questions about polymer crystallisation to be tackled precisely. Molecular dynamics (MD) simulations can provide insights but studying large lamellar structures is challenging. Meyer and Muller-Plathe set the stage for molecular dynamics (MD) simulations of large lamella structures, by demonstrating that reproducing local crystalline structures is unimportant when large crystalline and amorphous regions dominate properties. Here, the role of short chain branches (SCBs) (C4) on the melt and crystalline properties of monodisperse polyethylene systems (C400) is investigated, using CGMD simulations. SCBs are grown into the melt to minimise computational expense, providing access to large systems. Cooling and heating cycles reveal the crystalline morphology depends strongly on both cooling rate and number of branches. Bidisperse mixtures of ultra-long C4000 and C400 are also studied, with different branch distributions, which mimic industrial PE morphologies. Via self-seeding, well aligned lamella are grown and morphological features, i.e. tie chains analysed. We begin to address how these features influence crystalline structure and material properties. We thank TotalEnergies for funding and GENCI/IDRIS (Orsay) and CAIUS/HPC centre.

CPP 41.4 Thu 16:00 H39

Aggregation and ordering in small alkane systems — •Timur Shakirov and Wolfgang Paul — University of Halle, Halle, Germany

Ordering of small alkanes differs drastically from the bulk one. The difference is not only quantitative but also qualitative: short-chain single alkanes fold at low temperatures into non-trivial structures [1] in contrast to fully-stretched-chain lamellae in bulk. For the few chain systems we demonstrate the leading role of torsional stiffness in the ordered structure formation and investigate the corresponding conformations, which vary from spirals to tilted lamellae. For the fully stretched chain lamellae we find a two-step ordering, the indications of which remain at least up to 16 chain aggregates. In contrast to the low-temperature ordering, the aggregation or liquid-vapor transition leads to similarly disordered structures for all system sizes, which allows correction of size effects and extrapolation of the estimated aggregation temperatures to the thermodynamic limit. Our calculations of aggregation/boiling temperatures at normal pressure are in good agreement with experimental data. The presented equilibrium results 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 et al, 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 41.5 Thu 16:15 H39

How the competition between crystal growth and intracrystalline chain diffusion determines the lamellar thickness in semicrystalline polymers — Martha Schulz, Mareen Schäfer, Kay Saalwächter, and •Thomas Thurn-Albrecht — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle

The non-equilibrium thickness of lamellar crystals in semicrystalline polymers varies significantly between different polymer systems and depends on the crystallization temperature T_c. There is currently no consensus on the mechanism of thickness selection. Previous work has highlighted the decisive role of intracrystalline chain diffusion (ICD) in special cases, but a systematic dependence of lamellar thickness on relevant timescales such as that of ICD and stem attachment has not yet been established. Studying the morphology by small-angle X-ray scattering and the two timescales by NMR methods and polarization microscopy, we present data on poly(oxymethylene), a case with relatively slow ICD. It fills the gap between previously studied cases of absent and fast ICD, enabling us to establish a quantitative dependence of lamellar thickness on the competition between the noted timescales. Ref. Nature Communications, 13.1 (2022): 1-10.

15 min. break

CPP 41.6 Thu 16:45 H39

The Crucial Role of Solvation Forces in Inter-Nanoplatelet Interactions and Stack Formation — •Nanning Petersen, Martin Girard, Andreas Riedinger, and Omar Valsson — Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz

Cadmium selenide nanoplatelets show the tendency to form stacks in apolar alkane solvents. This effect is very similar to the stack formation of micron-sized discs, which can be induced by depletion forces. However, the interplay of the various forces leading to stack formation of nanoplatelets remains unclear. Solvation forces are in their origin and behaviour very similar to depletion forces.

Here, we use coarse-grained molecular dynamics simulations of nanoplatelets in octane solvent to investigate the role of solvation forces in nanoplatelet interactions. We demonstrate that solvation forces resulting from solvent layering are sufficiently strong to stabilize nanoplatelet stacks. We examine the dependence of solvation forces on the nanoplatelets' ligand shell, size, and other parameters. In particular, we demonstrate that for sufficiently large nanoplatelets, solvation forces are proportional to the interacting facet area, and their strength is intrinsically tied to the softness of the ligand shell. The solvation forces exhibit an oscillatory nature; increases in their strength leads to a stronger attraction between close nanoplatelet facets and in addition to an increase in the kinetic barriers.

[1] N. Petersen , M. Girard, A, Riedinger, and O. Valsson, ChemRxiv, doi:10.26434/chemrxiv-2022-mw1cs (2022)

CPP 41.7 Thu 17:00 H39

In situ small-angle X-ray scattering and total scattering to study CuPd nanoparticle growth and self-assembly — •Kilian Frank[1], Davide Derelli[2], Dorota Koziej[2], and Bert Nickel[1] — [1]Faculty of Physics and Center for Nanoscience (CeNS), Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Germany — [2]University of Hamburg, Institute for Nanostructure and Solid-State Physics, Center for Hybrid Nanostructures, 22761, Hamburg, Germany

Combining noble metals with abundant materials is a promising design strategy for new catalytic nanomaterials, e.g. for CO_2 reduction. Reliable synthesis routes of nanoparticles with a low size dispersity are required, but often an understanding of the formation pathway is lacking. Therefore, we investigated the entire synthesis of CuPd alloy nanoparticles using simultaneous small-angle X-ray scattering (SAXS) and the atomic pair distribution function obtained from total scattering (TS) to establish the sequence of structures from the atomic level to the nanoscale. We use a dedicated reaction cell for heating and stirring at the high-energy beamline P07 (PETRA III, DESY), extending our previous studies on cobalt oxide nanoparticle formation (https://doi.org/10.1038/s41467-021-24557-z). We characterize the transformation of precursors and early nucleation by TS, and the subsequent particle growth and assembly by SAXS in a model-based analysis. Upon cooling, we observe a rich temperature-dependent phase behavior of particle assemblies. These can serve as a potential templating strategy for efficient particle-based catalysts.

CPP 41.8 Thu 17:15 H39

Ligand-stabilized gold nanorods as an ideal model system for anisotropic colloids — •Marcel Krüsmann and Matthias Karg — Physikalische Chemie I: Kolloide und Nanooptik, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, 40225, Germany

Anisotropic colloidal particles have interesting optical, electronic and self-assembly properties. Yet the investigation of their phase behavior is often difficult due to limitations in quantity, monodispersity and colloidal stability for many particles. An additional challenge is the precise determination of particle number concentrations.

The easily scalable synthesis of gold nanorods gives access to monodisperse anisotropic colloids with a broad range of aspect ratios. The functionalization of gold nanorods with a polymer ligand increases the colloidal stability and removes the large excess of surfactant that is most often used in particle synthesis.

These anisotropic particles can now be studied with various methods. One of this methods is small-angle X-ray scattering for which gold has an excellent contrast. In combination with the good colloidal stability it is now possible to not only study the form factor but also the structure factor at high concentrations and/or during induced aggregation. The addition of absolute intensity measurements gives access to the particle number concentration, that can be related to measured extinction from spectroscopy.

CPP 42: Perovskite and Photovoltaics 5 (joint session HL/CPP/KFM)

Time: Thursday 15:00–16:30 Location: H31

CPP 42.1 Thu 15:00 H31

Atomically Thin Sheets of Lead-Free 1D Hybrid Perovskites Feature Tunable White-Light Emission from Self-Trapped Excitons — •Philip Klement[1], Natalie Dehnhardt[2], Chuan-Ding Dong[3], Florian Dobener[1], Julius Winkler[2], Samuel Bayliff[4], Detlev M. Hofmann[1], Peter J. Klar[1], Stefan Schumacher[3,5], Sangam Chatterjee[1], and Johanna Heine[2] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Marburg, Germany — [3]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Paderborn, Germany — [4]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, OK, USA — [5]College of Optical Sciences, The University of Arizona, Tucson, AZ, USA

One of the major current challenges in 2D materials' synthesis is the intentional design of building blocks to introducing superior chemical and physical properties. The limiting factor in this approach is the commonly-believed paradigm that in-plane covalent interactions are strictly necessary to form 2D materials, limiting the number of candidates. Here, we go beyond the paradigm that atomically thin materials require in-plane covalent bonding and report single layers of the one-dimensional organic-inorganic perovskite [C7H10N]3[BiCl5]Cl. Its unique 1D-2D structure enables single layers and the formation of self-trapped excitons which show white-light emission.

CPP 42.2 Thu 15:15 H31

Multiple spin-flip Raman scattering in bulk lead halide perovskites — •Marek Karzel[1], Dennis Kudlacik[1], Natalia E.

Kopteva[1], Ina Kalitukha[2], Maksym V. Kovalenko[3], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]St. Petersburg, Russia — [3]Laboratory of Inorganic Chemistry, ETH Zürich, 8093 Zürich, Switzerland

Lead halide perovskites like FACs are promising competitors for conventional semiconductors in spintronics due to their highly efficient light absorption and emission properties. We study spin-flip Raman scattering (SFRS) of resident carriers and investigate possible carrier exchange interactions. The measurements are performed at low temperatures around 1.6 K and external magnetic fields up to 10 T in Faraday and tilted geometries. This method allows us to observe Raman shifts in high magnetic fields which according to [1] are attributed to the g-factors of resident electrons and holes. The SFRS efficiency significantly increases for resonant probing of the free exciton resonances. We conduct from our measurements, that the creation of the free exciton is the essential requirement for observation of multiple spin-flip Raman scattering.

[1] E. Kirstein et al., Adv. Mater. 34, 2105263 (2022).

CPP 42.3 Thu 15:30 H31

Stability Enhancement of perovskite nanoplatelets via crosslinking of ligands — •Maximilian Gruber, Ulrich Leo, Nina Henke, Patrick Ganswindt, Michael Lichtenegger, Connor Heimig, and Alexander Urban — Nanospectroscopy Group and Center for Nanoscience (CeNS), Nano-Institute Munich, Department of Physics, Ludwig-Maximiliāns-Universitat München, Königinstr. 10, 80539 Munich, Germany

In recent years lead halide perovskite nanoplatelets (NPL) have attracted a lot of attention due to low-cost production and excellent spectral tuning. Additionally, perovskite NPLs exhibit the benefit of exciton energy tunability via quantum confinement as well as large photoluminescence quantum yield. The high surface to volume ratio of the NPLs, however, makes them susceptible to degradation by water, air and ion migration.

One solution to these issues of degradation investigated here is a process called crosslinking. Hereby the exposure of a film of NPLs to a dose of electron radiation induces intermolecular bonds between the organic ligands attached to the individual nanocrystals, hence forming a protective matrix around a film of pristine perovskite NPLs.

Varying dosages of irradiation of three monolayer CsPbBr3 NPLs were investigated followed by an exposure to other halides, NPLs with a different halide composition as well as different solvents, showing a drastic increase in stability of the crosslinked compared to untreated NPLs. This enables the possibility of a future application of lead halide perovskite NPLs under ambient conditions.

CPP 42.4 Thu 15:45 H31

Enhancing the optical performance of perovskite nanoplatelets — •Stefan Martin[1], Carola Lampe[1], Nina Henke[1], Ioannis Kouroudis[2], Milan Harth[2], Alessio Gagliardi[2], and Alexander Urban[1] — [1]LMU Munich, Nanospectroscopy Group — [2]TU Munich

Lead halide perovskites have been drawing a lot of interest during the last few years due to their unique properties. Their excellent optical performance combined with easy and cost-efficient production are interesting for both light-emitting devices and solar cells. Perovskite nanoplatelets are furthermore convincing with high photoluminescence quantum yields and narrow emission linewidths tunable from 430 to 505 nm. The thickness of these nanoplatelets can be tuned with a monolayer precision and determines the absorption and emission profile of the sample.

By using different machine learning approaches the synthesis parameters were investigated and optimized based on the emission spectrum. With this method, the emission properties of nanoplatelets with thicknesses reaching from 2 to 8 monolayers were enhanced. Additionally, the emission wavelengths can be finetuned using a post-synthetic enhancement treatment comprising a lead halide ligand solution. Depending on the time interval between synthesis and enhancement, a redshift of controllable extent can be introduced while further reducing the emission linewidth. With these strategies, a narrow and symmetric emission peak can be achieved at any desired wavelength. This is particularly interesting for the implementation in optoelectronic devices.

CPP 42.5 Thu 16:00 H31

Extensive study on sequential physical vapor deposition of mixed-cation perovskite (Cs,FA)PbI_3 — •Karl Heinze[1], Tobias Schulz[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, von-Danckelmann-Platz 3, 06120 Halle (Saale), Germany — [2]Universidad de Pablo Olivade, Carretera de Utrera 1, 41013, Sevilla, Spain

Sequential deposition via physical vapor deposition (PVD) is underexplored, even though it offers precise adjustment of components and composition and a variety of routes to investigate the optimization of perovskite growth. We combine in situ XRD and in situ laser light scattering to monitor phase evolution of (Cs,FA)PbI3 during PVD. We study the influence of deposition sequence of the components PbI2, FAI and CsI on CsFAPbI3 growth. Noticeably, the sequence strongly influences the orientation of deposited components. Similarly, diffusion before and during annealing as well as resulting alpha phase share depend on the evaporation sequence. When depositing PbI2 first, conversion to the perovskite phase was not achieved, unless an over stoichiometric share of FAI was deposited. Depositing FAI first and PbI2 later resulted in a high probability of layer conversion to the perovskite phase without secondary phases being detected. A striking feature during our investigation was the absence of the delta phase during deposition and annealing, seemingly caused solely by the preparation method. We deliver important insight into this poorly investigated preparation path and provide a foundation for further research based on our detailed study of sequence-dependent crystalline growth.

CPP 42.6 Thu 16:15 H31

Ultrafast transient spectroscopy of Cu(In,Ga)Se_2 coupled to different buffer layers. — •Pirmin Schweizer, Ricardo Rojas-Aedo, Alice Debot, Philip Dale, and Daniele Brida — Department of Physics and Materials Science, University of Luxembourg, 162a avenue de la Faïencerie, L-1511 Luxembourg, Luxembourg

The dynamic parameters of photo-induced electron-hole pairs, such as recombination time and charge conductivity, play a major role in the efficiency of photovoltaic devices. Among thin film materials for photovoltaics, one of the most interesting is the p-type Cu(In,Ga)Se_2 alloy (CIGS) on which an n-type buffer layer is deposited, forming the initial part of the device p-n junction. The inter-material transport dynamics strongly depend on how the band structure is affected by the buffer layer, and also on the quality of the CIGS \ buffer layer interface which may contain defects. In our experiments we have compared the ultrafast transient reflectivity on CIGS epitaxially grown on a GaAs substrate. New Cd free buffer layers In_2S_3 and band offset tunable Zn(O,S), are compared to the most commonly used buffer layer, CdS. The transient reflection measurements allows for the extraction of the electronic transport dynamics at the interface with the buffer. This study allows us to draw conclusions about the pair formation capacity mediated by the transport properties between the CIGS and the buffer layer. The results can guide the development of Cd free buffer layers thus reducing the environmental impact caused by CdS in traditional CIGS solar cells.

CPP 43: Members' Assembly

Time: Thursday 18:00–19:00 Location: H39

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 44: Focus Session: Soft Matter and Nanocomposites: New Opportunities with Advanced Neutron Sources 2

organized by Stephan Förster (FZ Jülich), Thomas Gutberlet (FZ Jülich), Peter Müller-Buschbaum (TUM) and Walter Richtering (RWTH Aachen)

Time: Friday 9:30–11:15 Location: H38

Invited Talk CPP 44.1 Fri 9:30 H38

Connecting dynamics and phase behavior of proteins: The neutron perspective — •Frank Schreiber — Universität Tübingen, Germany

We discuss the combination of various neutron scattering techniques to shed light on the dynamics of proteins in aqueous solution. This includes several processes, such as backbone and side-chain fluctuations, interdomain motions, as well as global rotational and translational (i.e. center of mass) diffusion. Since protein dynamics is related to protein function and essential transport processes, a detailed mechanistic understanding and monitoring of protein dynamics in solution is highly desirable. In particular, we connect it to the overall phase behavior in terms of clustering, crowding, crystallization, and phase separation [1], employing a combination of elastic, quasi-elastic, and inelastic scattering [2] as well as complementary techniques, such as X-ray photon correlation spectroscopy (XPCS) and simulations [3]. Finally, we comment on future perspectives with advanced neutron sources. Invaluable contributions by numerous collaborators are gratefully acknowledged.

[1] M. Grimaldo et al., JPCL, 10, 1709 (2019) [2] M. Grimaldo et al., Quarterly Reviews of Biophysics, 52, e7 (2019) [3] A. Girelli et al., Phys. Rev. Lett. 126 (2021) 138004

CPP 44.2 Fri 10:00 H38

Self-assembly of supramolecular magnetic polymers with monomers of different sizes — Ekaterina Novak[1], Elena Pyanzina[1], •Marina Gupalo[1], and Sofia Kantorovich[1,2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

In this paper we studying the effect of polydispersity of magnetic particles on the self-assembly of supramolecular magnetic polymers. Magnetic polymers are widely used to create new magnetically controlled materials and represent an analogue of polymer chains, where polymer molecules serve as crosslinks, and magnetic particles replace monomers. We propose to consider the bidisperse model, which takes into account only two fractions of particles in size, which is enough to track the main influence of polydispersity on the self-organization of a magnetic polymer. Using the method of computer simulation of Langevin's dynamics, we study various structural parameters of an individual magnetic polymer of different configurations: a chain, a closed ring, an X-shaped and Y-shaped magnetic filament. For analysis of the qualitative changes in equilibrium properties with temperature were used radius of gyration and magnetic moment, the general microstates are also defined. It turned out that the considered new types of polymer configuration compared with the monodisperse model significantly affect the equilibrium properties. This work was supported by RSF grant 19-72-10033.

CPP 44.3 Fri 10:15 H38

Pathways of micellar collapse and swelling of PMMA-*b*-PNIPAM in aqueous solution after a rapid change of pressure — •Pablo A. Alvarez Herrera[1], Johannes Allwang[1], Feifei Zheng[1], Cristiane Henschel[2], Leonardo Chiappisi[3], Alfons Schulte[4], André Laschewsky[2], and Christine M. Papadakis[1] — [1]TU München, Physik-Department, Garching, Germany — [2]Institut für Chemie, Potsdam-Golm, Germany — [3]Institut Laue- Langevin, Grenoble, France — [4]University of Central Florida, Orlando, USA

In aqueous solution, diblock copolymers consisting of a permanently hydrophobic and a thermo-responsive block can self-assemble into different morphologies. In particular, poly (methyl methacrylate)-*b*-poly(*N*-isopropylacrylamide) (PMMA-*b*-PNIPAM) forms spherical micelles featuring a PMMA core and a thermo-responsive PNIPAM shell. At atmospheric pressure, the micellar shell dehydrates, and the collapsed micelles form aggregates when heating above the cloud point of PNIPAM [1]. This phase transition can be also induced by changing the pressure. In this contribution, we study the micellar collapse and their posterior aggregation by kinetic small-angle neutron scattering (SANS) in combination with rapid pressure jumps across the co-existence line. The disintegration of the aggregates and the micellar swelling are also investigated by performing the pressure jump in the opposite direction.

[1] C.-H. Ko, C. M. Papadakis et al., Macromolecules 54, 384 (2021).

CPP 44.4 Fri 10:30 H38

Investigation of the Effect of Magnesium Salts with Chaotropic Anions on the Swelling Behavior of PNIPMAM Thin Films — •Julija Reitenbach[1], Christina Geiger[1], Peixi Wang[1], Robert Cubitt[2], Dirk Schanzenbach[3], André Laschewsky[3], Christine M. Papadakis[4], 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 — [4]TU München, Physik-Department, Physik weicher Materie, 85748 Garching

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 the polymer chains 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.

Invited Talk CPP 44.5 Fri 10:45 H38

Magnetic particle self-assembly at functionalized interfaces — •Max Wolff — Department for Physics and Astronomy, Uppsala University, Uppsala, Sweden

Neutrons allow the study of buried interfaces and are directly sensitive to magnetic induction. This makes grazing incidence neutron scattering an ideal tool for the study of self-assembled magnetic particles.

In this talk I will discuss the self-assembly of monodisperse colloidal magnetite nanoparticles from a dilute water-based ferrofluid onto functionalized silicon surfaces. The density of the layer adjacent to the substrate is determined by the interaction between the particles and the substrate. Dense layers form for chemical binding and magnetic substrates, while less dense and no layering is found for physisorption and repulsive interactions. Once adsorbed subsequent layers assemble due to magnetic dipolar forces. The layering gets more pronounced for larger dipole moments of the particles. Once formed the density and structure of the layers may be tuned by magnetic and/or shear fields.

Magnetic particles may also be used to self-assemble polymer micelles. Applied magnetic fields may result in a micro shear effect aligning the domains of micellar crystals. By stroboscopic reintegration this reorientation process may be followed on time scales down to ms and resonant enhancement may aid the identification of off-specular and grazing incidence small angle scattering.

CPP 45: Biopolymers, Biomaterials and Bioinspired Functional Materials (joint session CPP/BP)

Time: Friday 9:30–11:15 Location: H39

Invited Talk CPP 45.1 Fri 9:30 H39

New biobased material concepts using scattering techniques to elucidate and control nanoscale assembly — •Daniel Söderberg — KTH Royal Institute of Technology, Department of FIbre and Polymer technology, Stockholm, Sweden

Cellulose, the most abundant biopolymer on earth, can be crucial in mitigating fossil-based resources to more sustainable solutions. It is used as an engineering material, e.g. sawn timber, pulp for papermaking or as a polymer as a basis for plastic materials.

Cellulose nanofibres (CNF) constitute the structural component of plants, it is a semi-crystalline, semi-flexible rod-like nanoparticle having cross-sections in the order of 4-5 nm and lengths around one micrometre. Based on technical developments during the last decades, it is today possible to extract the CNF in large quantities, which has promoted significant research efforts aiming at new material concepts and devices based on cellulose.

Small and wide-angle x-ray scattering have been used to understand nanoscale assembly during fibre spinning from a CNF dope using microfluidics, allowing the tuning of the hierarchical structure, resulting in 100% bio-based filaments with exceptional properties. Furthermore, to develop scalable engineering processes, an in-depth understanding of nanoscale diffusion and the effects of nanoparticle interaction in low-concentration crowded systems has been pursued by combining light-scattering, X-ray Photon Correlation Scattering and coarse-grain modelling.

CPP 45.2 Fri 10:00 H39

A Semisynthetic Superparamagnetic Nanoprobe for Protein Targeting and Manipulation — •Andreas Neusch[1], Iuliia Novoselova[1], Nikolaos Tetos[2], Michael Farle[2], Ulf Wiedland[2], and Cornelia Monzel[1] — [1]Heinrich-Heine University Düsseldorf, Germany — [2]University of Duisburg-Essen, Germany

Probing and manipulating biological functions requires tools to target and modify the proteins involved in the respective process. In recent years Magnetogenetics emerged as an approach where magnetic nanoparticles (MNPs) and external magnetic fields are used to realize such manipulation (Lisse et al., Adv. Mater., 29, 1700189 (2017)). The advantages of this combination lies within the deep tissue penetration of magnetic fields and the possibility to apply stimuli on nanoscales leading to spatial redistribution, force application, or heat generation of proteins. However, a precise active perturbation requires MNPs to be monodisperse, biocompatible, tunable with regard to their magnetic properties, as well as exhibiting a modifiable molecular shell (Monzel et al., Chem. Sci. 8, 7330-7338 (2017)). Here, we synthesize a bioinspired semisynthetic MNP - Magnetoferritin (MFt) -, which fulfils these demands. MFt is based on the globular iron storage protein complex ferritin that converts iron ions to a ferrihydrite core but can be synthetically loaded with a magnetic iron oxide core (Novoselova et al., Nanomaterials, 11, 2267 (2021)). MFt was chemically, physically and magnetically characterized both in vitro and in vivo. We demonstrate how MFt can be used to target proteins on living cells as well as to spatially manipulate MFts in a single cell environment.

CPP 45.3 Fri 10:15 H39

Bioinspired electrodes for brain wave detection — •Volker Körstgens[1], Gökay Erbil[1], Andreas Zheng[1], Hsin-Yin Chiang[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]Cephalgo, 67000 Strasbourg, France

With increasing demands in brain computer interfaces (BCI) measuring biosignals non-invasively becomes more important. Applications like measuring brain waves via electroencephalography (EEG) with dry electrodes remains challenging as for a steady biosignal acquisition adhesion to the skin has to be maintained all the time. We present two different approaches inspired by nature for such electrodes. In our first approach we developed micro-structured dry adhesive electrodes based on polydimethylsiloxane (PDMS) with conductive fillers. The EEG-performance and adhesive properties of these electrodes will be discussed and compared to the concept of mussel-inspired hydrogels we follow in our second approach.

CPP 45.4 Fri 10:30 H39

Anionically functionalized glycogens efficiently encapsulate cationic peptides — Hanna Zhukouskaya[1], •Pablo M. Blanco[2], Zulfiya Černochová[1], Lucie Čtveráčková[1], Roman Staňo[3], Ewa Pavlova[1], Miroslav Vetrík[1], Peter Černoch[1], Miroslav Šlouf[1], Marcela Filipová[1], Miroslav Štěpánek[2], Martin Hrubý[1], Peter Košovan[2], and Jiří Pánek[1] — [1]Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Prague 6, Czech Republic — [2]Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Hlavova 8, 128 40 Prague 2, Czech Republic — [3]Faculty of Physics, University of Vienna, Kolingasse 14-16, 1090 Vienna, Austria

We developed and tested novel acid-functionalized glycogen conjugates as supramolecular carriers for efficient encapsulation and inhibition of a model cationic peptide melittin, which is the main component of honeybee venom. Systematic investigation of this model system allowed us not only to test its potential application as honeybee venom antidote but also to assess the role of the degree of substitution and solution pH in the interactions of these anionic carriers with multivalent cationic cargos. Our results demonstrate that the concept of electrostatically driven encapsulation by acid-functionalized glycogens should be applicable not only to the model case of melittin but also to other multivalent cationic biomolecules.

CPP 45.5 Fri 10:45 H39

Dissipative Assembly: Controlling Changes of Membrane Topology by Reaction Cycles — •Gregor Ibbeken and Marcus Müller — Institut für Theoretische Physik, Georg-August Universität, Friedrich-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 polymers which can switch between a hydrophilic and an amphiphilic state and in the latter self-assemble to form vesicles in aqueous solution. This can occur either by macromolecular or monomeric reactions. In both cases a precursor reacts with a fuel to a product, which itself can decay back to the precursor. We perform particle-based simulations using a soft, coarse grained model for polymers. For the macromolecular reactions we find two drastically different scenarios depending on the fuel volatility: (i) For high fuel volatility, the coupling of inactivated to activated polymers introduces a length scale which dictates the maximal vesicle size and prevents fusion beyond this. This results in an interplay between the architecture- and the reaction-rate-determined length and time scales. (ii) For less volatile fuel, a fuel gradient arises in the system. This results in the compartments moving within the fuel gradient to approach the source. In doing so the moieties gain material over long times which drastically changes the formation mechanism of the vesicles. Finally, we show that the above reaction mechanism can be mimicked by monomeric reactions by the use of multiple, inhomogeneously distributed fuels.

CPP 45.6 Fri 11:00 H39

Influence of molecular weight of polycation polydimethyldiallylammonium and carbon nanotube content on the electric conductivity of layer-by-layer films — •Sven Neuber[1], Annekatrin Sill[1], Peter Nestler[2], Heiko Ahrens[1], and Christiane A. Helm[1] — [1]Universcity of Greifswald, Institut of Physics, Greifswald, Germany — [2]TÜV NORD EnSys GmbH & Co. KG, Greifswald, Germany

For biological and engineering applications, nm-thin films with high electrical conductivity and tunable sheet resistance are desirable. Multilayers of polydimethyldiallylammonium chloride (PDADMA) with two different molecular weights (322 and 44.3 kDa) and oxidized carbon nanotubes (CNTs) were constructed using the layer-by-layer technique. Both the film thickness and the surface coverage of the CNTs increased linearly with the number of CNT/PDADMA bilayers deposited (dfilm up to 80 nm). Atomic force microscopy images showed a predominantly surface-parallel orientation of CNTs. Ohmic behavior with constant electrical conductivity of each CNT/PDADMA film and conductivity up to 4*10^3 S/m was found. A change in PDADMA molecular weight by almost a factor of ten does not affect the film thickness and electrical conductivity, only the film/air roughness is reduced. However, increasing CNT concentration in the deposition dispersion from 0.15 up to 0.25 mg/ml results in an increased thickness of a CNT/PDADMA bilayer (by a factor of three). The increased bilayer thickness is accompanied by a decreased CNT coverage and a decreased electrical conductivity (by a factor of four).

CPP 46: 2D Materials 10 (joint session HL/CPP/DS)

Time: Friday 9:30–12:00 Location: H36

CPP 46.1 Fri 9:30 H36

THz conductivity of nanograined Bi2Te3 pellets with varying Te doping — •Ahana Bhattacharya[1], JeongWoo Han[1], Sepideh Izadi[2], Sarah Salloum[3], Stephan Schulz[3], Gabi Schierning[2], and Martin Mittendorff[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Universität Bielefeld, Fakultät für Physik, 33615 Bielefeld, Germany — [3]Universität Duisburg-Essen, Fakultät für Chemie, 45141 Essen, Germany

The topological insulator Bi2Te3 hosts surface states with a high carrier mobility as back scattering of charge carriers is suppressed due to the spin-momentum locking. While in large crystals the electronic properties are dominated by the bulk states, hot-pressed pellets of nanograined Bi2Te3 offer a high surface-to-volume ratio, which provides a platform to exploit the surface carriers even in extended samples. Here we employ THz time-domain spectroscopy to disentangle the contribution of surface and bulk carriers to the transport properties. Even at room temperature the THz reflection is determined by characteristic features of the high-mobility surface carriers, i.e. Drude conductivity but also plasmonic contributions. The latter are caused by confinement of the surface carriers due to the mechanical structure of the sample. Variations of the Te content allows to shift the Fermi energy and thus strongly influences the resulting THz spectra.

CPP 46.2 Fri 9:45 H36

Direct growth of monolayer MoS2 on nanostructured silicon waveguides — •A Kuppadakkath[1], E Najafidehaghani[2], Z Gan[2], A Tuniz[3], G Ngo[1], H Knopf[1], F Löchner[1], F Abtahi[1], T Bucher[1,5], S Shradha[1], T Käsebier[1], S Palomba[3], N Felde[4], P Paul[1], T Ullsperger[1], S Schröder[4], A Szeghalmi[1,4], T Pertsch[1,4], I Staude[1,5], U Zeitner[1,4], A George[2], A Turchanin[2], and F Eilenberger[1] — [1]Institute of Applied Physics (FSU), Jena, Germany — [2]Institute of Physical Chemistry (FSU), Jena, Germany — [3]Sydney Nano, Camperdown, Australia — [4]Fraunhofer IOF, Jena, Germany — [5]Institute of Solid State Physics (FSU), Jena, Germany

We report for the first time the direct growth of Molybdenum disulfide (MoS2) monolayers on nanostructured silicon-on-insulator waveguides. Our results indicate the possibility of utilizing the Chemical Vapour Deposition (CVD) on nanostructured photonic devices in a scalable process. Direct growth of 2D material on nanostructures rectifies many drawbacks of the transfer-based approaches. We show that the van der Waals materials grow conformally across the curves, edges, and the silicon-SiO2 interface of the waveguide structure. Here, the waveguide structure used as a growth substrate is complex not just in terms of its geometry but also due to the two materials (Si and SiO2) involved. A transfer-free method like this yields a novel approach for functionalizing nanostructured, integrated optical architectures with an optically active direct semiconductor.

CPP 46.3 Fri 10:00 H36

Atomic layer deposition of ternary MoWS$_2$ — •Christian Tessarek, Tim Grieb, Andreas Rosenauer, and Martin Eickhoff — Institut für Festkörperphysik, Universität Bremen

Two-dimensional (2D) monolayers of binary molybdenum disulfide (MoS$_2$) and tungsten disulfide (WS$_2$) belong to the transition metal dichalcogenide (TMDC) material family and are direct band gap semiconductors. The optical band gap of monolayer MoS$_2$ and WS$_2$ is $\sim$1.9 and 2.0 eV, respectively. Ternary Mo$_x$W$_{1-x}$S$_2$ enables tuning of excitonic transition energy dependent on the concentration x.

Atomic layer deposition (ALD) is used to deposit MoWS$_2$ in the whole composition range between pure MoS$_2$ and WS$_2$. The concentration x is determined by the frequency position of the A$_{1g}$ Raman mode. The distribution of W and Mo atoms in the crystal lattice of MoWS$_2$ is studied by high resolution scanning transmission electron microscopy. Additional annealing is performed to improve structural and optical properties. Photoluminescence spectroscopy measurements show concentration dependent spectral position of A and B excitonic emission.

CPP 46.4 Fri 10:15 H36

Epitaxial growth of post transition metal chalcogenides: From standard approaches to new capabilities — •Eugenio Zallo[1,2], Michele Bissolo[1], Marco Dembecki[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter-Schottky-Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748, Garching, Germany — [2]Paul-Drude-Institut für Festkoerperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117, Berlin, Germany

Van der Waals (vdW) materials grown epitaxially are an urgent challenge for the development of scalable and high-crystalline-quality semiconductor films that can be exploited for novel device technologies. 2D materials "beyond graphene" have sparked immense interest in recent years, due to their excellent physical properties. Among them, post transition metal chalcogenides (PTMC, M={In,Ga} and C={S,Se,Te}) are vdW semiconductor materials with extraordinary photoresponsivity, a quasi-direct gap with a Mexican hat valence band and promising thermoelectric properties but they suffer from fast layer oxidation. In this presentation, the molecular beam epitaxy (MBE) growth of large-area PTMC is demonstrated on 3D and 2D bonded substrates by means of encapsulation strategies and careful microscopic and spectroscopic characterizations supported by density functional theory calculations. In order to study the pristine information of air sensitive materials, we present a cutting edge UHV cluster tool for the synthesis of ultrapure 2D-PTMCs and their heterostructures. The potential directions will be described.

CPP 46.5 Fri 10:30 H36

Fabrication of Dielectric Mirrors and Microcavity Configurations for Light-Matter Coupling with Transition-Metal Dichalcogenides Heterostructures — •Chirag Palekar[1], Manan Shah[2], Fynn Kunze[2], Peter Klar[2], Stephan Reitzenstein[1], and Arash Rahimi-Iman[2] — [1]Institute of Solid State Physics, Technische Universität Berlin, D-10623, Germany. — [2]I. Physikalisches Institut und Zentrum für Materialwissenschaften, Justus-Liebig Universität Gießen, D-35392, Germany

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15 min. break

CPP 46.6 Fri 11:00 H36

Selective area growth of MoS$_2$ via CVD on patterned GaN-AlO$_x$ substrates — •Simon Wörle, Theresa Grünleitner, Alex Henning, and Ian Sharp — Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany

Two-dimensional (2D) transition metal dichalcogenides have attracted considerable attention due to their unique optoelectronic properties. For the application of 2D materials in semiconductor devices, the controlled and scalable synthesis of high-quality 2D materials is critical.

Here, we demonstrate the selective area growth of MoS$_2$ by chemical vapor deposition (CVD) on GaN substrates that were patterned with ultrathin aluminum oxide coatings created by low-temperature atomic layer deposition. Optical and scanning electron microscopy images show that mono- and few-layer MoS$_2$ flakes preferentially nucleate and grow directly on the (uncoated) GaN. Atomic force microscopy and Raman measurements further reveal the formation of triangular and star-like shaped multilayer MoS$_2$ crystals at the interfaces between GaN and AlO$_x$. Moreover, the observed fixed orientation of the triangular MoS$_2$ flakes with respect to the GaN substrate lattice indicates van der Waals epitaxy. By altering the CVD growth conditions, the density of deposited MoS$_2$ flakes can be tuned, resulting in the growth of either isolated MoS$_2$ nanosheets or continuous films, in the latter of which the individual flakes have coalesced.

The presented results mark an important step towards integrated MoS_2 based heterostructures for semiconductor device applications.

CPP 46.7 Fri 11:15 H36

Patterned growth of transition metal dichalcogenides monolayers and multilayers for electronic and optoelectronic device application — •Seung Heon Han[1], Ziyang Gan[1], Emad Najafidehaghani[1], Fatemeh Abtahi[2], Christof Neumann[1], Julian Picker[1], Tobias Vogel[2], Uwe Hübner[3], Falk Eilenberger[2], Antony George[1], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Germany — [3]Leibniz Institute of Photonic Technology (IPHT), Jena, Germany

We present a simple, large area, cost effective soft lithographic method for growth of high-quality two-dimensional transition metal dichalcogenides (TMDs). Initially, a liquid precursor (Na2MoO4 in aqueous solution) is patterned on the growth substrate using micro-molding in capillaries (MIMIC) technique. Subsequently, a chemical vapor deposition (CVD) step is employed to convert the precursor patterns to monolayer, few layers, or bulk TMDs, depending on the precursor concentration. The grown patterns were characterized using optical microscopy, atomic force microscopy, Raman spectroscopy, X-ray photoelectron spectroscopy, scanning electron microscopy, and photoluminescence spectroscopy to reveal their morphological, chemical, and optical characteristics. The applicability of the grown patterned TMDs were tested for application such as field effect transistors, photodetectors, and memtransistor devices.

CPP 46.8 Fri 11:30 H36

Conductive 2D MOFs in van-der-Waals heterostructures — •Jonas Pöhls[1], Zhiyong Wang[2], Renhao Dong[2], and Thomas Weitz[1] — [1]I. Physical Institute University of Göttingen, Göttingen, Germany — [2]Technical University of Dresden, Dresden, Germany

In conventional three-dimentional (3D) Metal-Organic Frameworks (MOFs) the electric conductivity is limited by the large separation of the metal centers by the organic ligands. Recent advantages in the synthesis of layered two-dimensional conjugated MOFs (2D c-MOFs) lead to a large improvement of the electronic properties, these materials allow a charge transfer along both interlayer (π-π-stacking) and intralayer (basal plane) directions [1]. In order to elucidate the underlying charge transport mechanisms in the 2D c-MOFs, we perform electronic characterizations of the films implemented in field-effect transistors under varying conditions. In addition to the improved properties of the 2D c-MOFs themselves, their 2D nature make them also a promising candidate for the fabrication of van-der-Waals heterostructures with other 2D materials like graphene, which could give access to a variety of interaction-driven effects. We present first results on the charge transport of 2D c-MOFs down to the size of single crystals as well as implemented in van-der-Waals heterostructures.

[1] Z. Wang et al. "Interfacial Synthesis of Layer-Oriented 2D Conjugated Metal*Organic Framework Films toward Directional Charge Transport", J. Am. Chem. Soc. (2021)

CPP 46.9 Fri 11:45 H36

Controlled Encapsulation of Monolayer MoS2 with Ultrathin Aluminium Oxide for Tunnel Contacts — •Sergej Levashov, Chenjiang Qian, Theresa Grünleitner, Jon J. Finley, Alex Henning, and Ian D. Sharp — Walter Shottky Institut, TUM, München, Deutschland

Two-dimensional (2D) semiconductors have unique optoelectronic properties that provide the opportunity to overcome current scaling and performance limits of semiconductor devices. To harness the full of potential of 2D materials, requires their seamless integration with bulk materials. In particular, contacting mono- and few-layer 2D semiconductors with metals is challenging since the deposition process may introduce defects impeding interfacial charge transport. Here we use low-temperature atomic layer deposition to encapsulate monolayer MoS_2 with a van der Waals bonded and ultrathin aluminium oxide (AlO_x) layer. The 18 Å thin AlO_x coating introduces additional charge carriers ($\sim 5\cdot 10^{12}$ cm^{-2}), while it also protects monolayer MoS_2 from defect creation during metallization. Microscratching of the AlO_x adlayer by contact mode atomic force microscopy and subsequent spectroscopic analysis demonstrate the reversibility of the charge transfer doping effect, indicating weak interaction. Importantly, current voltage measurements yielded a two-fold reduction in the contact resistance for MoS_2 field-effect transistors contacted with AlO_x interlayer. Overall, this work demonstrates the beneficial effect of the AlO_x adlayer for improving 2D device contacts and provides a scalable route to the damage-free integration of 2D semiconductors.

CPP 47: Active Matter 5 (joint session DY/BP/CPP)

Time: Friday 10:00–12:45 Location: H18

CPP 47.1 Fri 10:00 H18

Anomalous cooling and overcooling of active colloids — •Fabian Jan Schwarzendahl and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

The phenomenon that a system at a hot temperature cools faster than at a warm temperature, referred to as the Mpemba effect, has been recently realized for trapped colloids. Here, we investigate the cooling and heating process of a self-propelling active colloid using numerical simulations and theoretical calculations with a model that can directly be tested in experiments. Upon cooling activity induces a Mpemba effect and the active particle escapes an effective temperature description. At the end of the cooling process the notion of temperature is recovered and the system can exhibit even smaller temperatures than its final temperature, a surprising phenomenon which we refer to as activity-induced overcooling.

CPP 47.2 Fri 10:15 H18

Active Ornstein-Uhlenbeck model for self-propelled particles with inertia — •Gia Huy Philipp Nguyen, René Wittmann, and Hartmut Löwen — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany

Self-propelled particles, which convert energy into mechanical motion, exhibit inertia if they have a macroscopic size or move inside a gaseous medium, in contrast to micron-sized overdamped particles immersed in a viscous fluid. We have studied an extension of the active Ornstein-Uhlenbeck model, in which the self-propulsion is described by colored noise, to access these inertial effects affecting their translational motion [1]. In this talk, analytical solutions of the mean displacement, mean-squared displacement and velocity autocorrelation function will be discussed for a free active particle and in more general settings including an active dimer, a time-dependent mass and various external forces.

[1] G. H. P. Nguyen, R. Wittmann, H. Löwen, J. Phys.: Condens. Matter 34, 035101 (2021)

CPP 47.3 Fri 10:30 H18

A quantitative scattering theory of active particles — •Thomas Ihle[1], Rüdiger Kürsten[1], and Benjamin Lindner[2] — [1]Institute for Physics, University of Greifswald, Greifswald — [2]Institute for Physics, Humboldt University of Berlin, Berlin

We consider a particular model of self-propelled particles with Kuramoto-type alignment interactions. Starting from the N-particle Fokker-Planck equation we observe that the usual factorization Ansatz of the probability density, often called Molecular Chaos approximation, predicts a relaxation behavior which qualitatively disagrees with agent-based simulations. Therefore, we develop a scattering theory which resolves the time-evolution of the two-particle correlation function, i.e. goes beyond the mean-field approximation. The theory does not require input from agent-based simulations; it is self-consistent and leads to analytical expressions. We show that this theory predicts the relaxation behavior of the system and the transport coefficients with high precision in certain parameter ranges.

CPP 47.4 Fri 10:45 H18

Hierarchical self-organization in communicating polar active matter — •Alexander Ziepke[1], Ivan Maryshev[1], Igor S.

Aranson[2], and Erwin Frey[1] — [1]Ludwig-Maximilians-Universität München, München, Germany — [2]Pennsylvania State University, University Park PA, USA

Self-organization in active matter plays an important role for various biological and artificial systems. In numerous cases, inter-agent communication is a key mechanism for the formation and localization of critical structures, such as the fruiting body in Dictyostelium discoideum or aggregation clusters in quorum-sensing bacteria. Despite its importance, the specific role of communication and its interplay with self-propulsion remains largely unexplored.

We propose a model for communicating active matter that endows self-propelled polar agents with information processing and signal relaying capabilities. We show that information processing greatly enriches the ability of these systems to form complex structures, allowing them to self-organize through a range of different collective dynamical states at multiple hierarchical levels. This provides insights into the role of self-sustained signal processing for self-organization in biological systems and opens pathways for applications using chemically driven colloids or microrobots.

CPP 47.5 Fri 11:00 H18

Collective transport of microparticles by active cells — •Robert Grossmann[1], Kevin Meissner[1], Fernando Peruani[2], and Carsten Beta[1] — [1]University of Potsdam, Potsdam, Germany — [2]CY Cergy Paris Université, Cergy-Pontoise, France

Motivated by the challenge of targeted delivery of micron-sized objects, we investigate a novel type of bio-hybrid active matter, composed of motile cells acting as autonomously moving agents that transport passive cargoes. The transport process is a collective phenomenon: a bead can be lost by one cell and may picked up by another one, or multiple cells transport one bead together, thereby giving rise to an intermittent, stochastic stop-and-go dynamics. Combining experiment and active matter theory, we investigate the emerging transport properties of this system. We first deduce the waiting time distributions of active and passive transport episodes from experiments with the amoeba *Dictyostelium discoideum*: whereas the duration of actual transport phases – determined by the time that cells and cargoes are in contact – are exponentially distributed, the waiting time distribution for passive periods exhibits power-law characteristics which results from the search of cells looking for immobile colloids. We predict displacement distributions and the mean-squared displacement of colloids based on the statistics of waiting times and particularly point out a crossover from normal to subdiffusive scaling. These results provide the basis for the future design of cellular micro-carriers and for extending our findings to more advanced transport tasks in complex, disordered environments, such as tissues.

CPP 47.6 Fri 11:15 H18

Odd viscosity and active turbulence of hydrodynamic microrotors — •Joscha Mecke[1], Yongxiang Gao[2], Dirk G.A.L. Aarts[3], Alberto Medina[1], Gerhard Gompper[1], and Marisol Ripoll[1] — [1]Institute of Biological Information Processing, Forschungszentrum Jülich, Germany — [2]Institute for Advanced Study, Shenzhen University, China — [3]Department of Chemistry, University of Oxford, UK

Suspensions of rod-like silica colloids with a ferromagnetic head are considered in a rotating magnetic field applied parallel to a substrate. The magnetic moment is oriented perpendicular to the rod axis which implies a non-equilibrium vertical orientation to the substrate and synchronous spinning in the rotating field. We combine experiments and simulations to study the collective properties of these rotors. The hydrodynamic flows generated by the colloid rotations induce a cascade of translational motions in the neighbouring colloids. Thus, the rotors can be regarded as active matter with transport coefficients varying with local configuration and thus rotor density. The competition between hydrodynamic and steric interactions renders the translational dynamics non-monotonous in rotor density. The ensemble dynamics shows the emergence of eddies of various sizes reminiscent of turbulence. Furthermore, the rotor fluid is a realisation of a chiral active fluid with odd viscosity, that manifests itself in stress forces orthogonal to the direction of shear. In vortex flow, the stress acts like an effective pressure leading to density-vorticity correlations. Our experimental and numerical results are found to be in agreement.

CPP 47.7 Fri 11:30 H18

Two-temperature activity drives liquid-crystal and crystalline order in soft repulsive spherocylinders — •Jayeeta Chattopadhyay, Sindhana Pannir-Sivajothi, Kaarthik Varma, Sriram Ramaswamy, Chandan Dasgupta, and Prabal K. Maiti — Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India

We study the scalar activity induced phase separation and liquid crystal ordering in a system of Soft Repulsive Spherocylinders (SRS) of various aspect ratios (L/D). Activity was introduced by increasing the temperature of half of the SRS (labeled 'hot') while maintaining the temperature of the other half constant at a lower value (labeled 'cold'). The difference between the two temperatures scaled by the lower temperature provides a measure of the activity. We find that activity drives the cold particles through a phase transition to a more ordered state and the hot particles to a state of less order compared to the initial equilibrium state. For L/D = 5, the cold components of a homogeneous isotropic (I) structure acquire nematic (N) and, at higher activity, crystalline (K) order. Similarly, the cold zone of a nematic initial state undergoes smectic (Sm) and crystal ordering while the hot component turns isotropic. Interestingly, we observe liquid crystal ordering for the spherocylinders having aspect ratio below Onsager's limit. The hot particles occupy a larger volume and exert an extra kinetic pressure, confining, compressing and provoking an ordering transition of the cold-particle domains.

Ref:Phys. Rev. E104, 054610 (2021).

CPP 47.8 Fri 11:45 H18

Spontaneous trail formation in populations of communicating active walkers — Zahra Mokhtari[1], Robert I. A. Patterson[2], and •Felix Höfling[1,3] — [1]Dept. Mathematics and Computer Science, Freie Universität Berlin — [2]WIAS Berlin — [3]Zuse Institute Berlin

How do ants form long stable trails? Despite abundant evidence that trail formation in colonies of insects or bacteria originates in their sensing of and responding to the deposits of chemicals that they produce, there is no consensus on the minimum required ingredients for this phenomenon. To address this issue, here, we develop an agent-based model in terms of active random walkers communicating via pheromones, which can generate trails of agents from an initially homogeneous distribution [1]. Based on extensive off-lattice computer simulations we obtain qualitatively the non-equilibrium state diagram of the model, spanned by the strength of the agent-chemical interaction and the number density of the population. In particular, we demonstrate the spontaneous formation of persistent, macroscopic trails, and highlight some behaviour that is consistent with a dynamic phase transition. We also propose a dynamic model for few macroscopic observables, including the sub-population size of trail-following agents, which captures the early phase of trail formation. At high densities and for strong alignment, we observe that rotating clusters ("ant mills") are more stable than trails and can swallow them up.

[1] Z. Mokhtari, R. I. A. Patterson & F. Höfling, New J. Phys. **24**, 013012 (2022).

15 min. break

CPP 47.9 Fri 12:00 H18

Dynamics of microalgae in a porous environment — •Florian von Rüling, Liubov Bakhchova, Dmitry Puzyrev, Ulrike Steinmann, and Alexey Eremin — Otto von Guericke University Magdeburg, Germany

The navigation through complex environments is a task the microalgae *Chlamydomonas reinhardtii* are frequently confronted with in their natural habitats, where they encounter suspended and sedimented particles as well as rough surfaces. To investigate the motion in heterogeneous surroundings, we observe dilute and crowded active colloidal suspensions of *Chlamydomonas* in quasi-two-dimensional microstructured PDMS-channels. Arrays of cylindrical or elongated pillars with varying lattice spacing and obstacle orientation serve as artificial porous environments. The swimmer behaviour is characterised by means of velocity and orientation autocorrelation functions, trajectory straightness, velocity distributions and the reflection/transmission coefficients for the porous segments.

CPP 47.10 Fri 12:15 H18

Extending the active Phase Field Crystal model to describe motility-induced condensation and crystallization — •Max Philipp Holl[1] and Uwe Thiele[1,2] — [1]Institut für Theoretische Physik, Universität Münster — [2]Center for Nonlinear Science, Universität Münster

The passive conserved Swift-Hohenberg equation (or phase-field-crystal [PFC] model) corresponds to a gradient dynamics for a single order parameter field related to density [1]. It provides a microscopic continuum description of the thermodynamic transition between liquid and crystalline states. A recent extension allows one to investigate both, vapour-liquid and liquid-solid transitions [3]. We first discuss the bifurcation and phase structure of this passive, i.e., thermodynamic model. Our subsequently introduced extension of the standard active PFC model [2] is able to describe passive and active (motility-induced) vapour-liquid and liquid-solid transitions. This is shown through a bifurcation and phase analysis based on path continuation supplemented by time simulations.

[1] H. Emmerich, H. Löwen, R. Wittkowski, T. Gruhn, G. I. Tóth, G. Tegze, and L. Gránásy. Phase-field-crystal models for condensed matter dynamics on atomic length and diffusive time scales: an overview. Adv. Phys., 61:665-743, 2012 [2] A. M. Menzel and H. Löwen. Traveling and resting crystals in active systems. Phys. Rev. Lett., 110:055702, 2013 [3] Z.-L. Wang, Z. Liu, Z.-F. Huang, and W. Duan. Minimal phase-field crystal modeling of vapor-liquid-solid coexistence and transitions. Phys. Rev. Materials, 4:103802, 2020

CPP 47.11 Fri 12:30 H18

Engines driven by active fields — •Patrick Pietzonka[1] and Michael E. Cates[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom

On macroscopic scales, where trajectories of individual particles cannot be observed, active matter may appear like matter in thermal equilibrium. We discuss how the non-equilibrium character of active matter can nonetheless be revealed by using it as a working medium of engines delivering mechanical work in an isothermal environment. We focus on scalar active field theories such as the active model B as minimal continuum models for active matter undergoing a phase separation. The shape and chemical potential of droplets can be controlled through external potentials and activity patterns. We show how an asymmetric periodic activity pattern can drive a flow of active matter against an external force, thus acting as an autonomous engine. Moreover, we calculate and optimise the work that can be extracted by a cyclic engine that manipulates the activity and the potential landscape.

CPP 48: Electrical, Dielectrical and Optical Properties of Thin Films (joint session CPP/KFM)

Time: Friday 11:30–12:30 Location: H38

CPP 48.1 Fri 11:30 H38

Mechanical nanoscale polarization switching in ferroelectric polymer films — •Kathrin Dörr, Martin Koch, Diana Rata, and Robert Roth — MLU Halle-Wittenberg

Ferroelectric polymer films offer strong advantages like mechanical flexibility, biocompatibility, optical transparency and low-cost processing. However, their dielectric or piezoelectric performance is often inferior to that of oxide ferroelectric materials. Key to that is the electric dipolar order which is naturally lower in semicrystalline polymers than in crystalline ferroelectrics. We introduce the reorientation and alignment of the electric polarization in thin films utilizing the mechanical effect of an unbiased scanning force microscopy tip, providing a versatile tool for nanoscale domain writing [1]. Thin films (50 - 150 nm) of P(VDF-TrFE) (78:22) on graphite were prepared with dense (110)-oriented beta-phase lamellae randomly oriented in the film plane. Domain patterns with resolution down to 50 nm have been written with four (out of six possible) local polarization orientations. Written domains show excellent long-time stability. We discuss a ferroelastic origin of the mechanical polarization switching and make suggestions for how to utilize the domain patterns in thin film devices. [1] Adv. Electron. Mater. 2022, 2101416

CPP 48.2 Fri 11:45 H38

In-situ investigations of morphology degradation and oxidation level changes in EMIM DCA post-treated PEDOT:PSS thin films upon external influence — •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 — [2]ELETTRA, 34149 Basovizza TS, Italy — [3]MLZ, TU München, 85748 Garching

Nowadays thermoelectric generators are considered a promising technique for heat waste recovery as they enable a direct conversion of a temperature gradient into electrical power. Especially, organic thermoelectric polymers are attractive, owning some advantages like low cost, lightness and high mechanical flexibility, low or no toxicity, as well as a usually low thermal conductivity. In our work we show the positive effect of ionic liquid (IL) treatment on the thermoelectric properties, Seebeck coefficient and electrical conductivity, of semi-conducting PEDOT:PSS thin films. Furthermore with different in-situ experiments like GISAXS (grazing incidence small angle x-ray scattering), UV-Vis, and conductivity measurements we examine the inner film morphology and oxidation level changes upon operation at different ambient conditions.

CPP 48.3 Fri 12:00 H38

Improvement of TE properties of PEDOT:PSS films via DMSO addition and DMSO/salt post-treatment resolved from a fundamental view — •Suo Tu[1], Ting Tian[1], Anna-Lena Oechsle[1], Shanshan Yin[1], Xinyu Jiang[1], Wei Cao[1], Nian Li[1], Manuel A. Reus[1], Lennart K. Reb[1], Shujin Hou[2], Aliaksandr S. Bandarenka[2], Matthias Schwartzkopf[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1,4] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, Physik-Department, Physik der Energiewandlung und -speicherung, 85748 Garching — [3]DESY, 22607 Hamburg — [4]MLZ, TU München, 85748 Garching

The combination of DMSO-solvent doping and physical-chemical DMSO/salt de-doping in a sequence has been used to improve the thermoelectric PEDOT:PSS films. The initial DMSO-doping treatment induces a distinct phase separation by facilitating the aggregation of the PEDOT molecules. At the same time, the subsequent DMSO/salt de-doping post-treatment strengthens the selective removal of the surplus non-conductive PSS chains. Substantial alterations in the oxidation level, chain conformations, PEDOT crystallites and their preferential orientation are observed upon treatment on the molecular level. At the mesoscale level, the purification and densification of PEDOT-rich domains enable the realization of inter-grain coupling by the formation of the electronically well-percolated network. Thereby, both electrical conductivity and Seebeck coefficient are optimized.

CPP 48.4 Fri 12:15 H38

Exciton dynamics in surface-mounted metal-organic frameworks: A femtosecond transient absorption study — •Vipilan Sivanesan[1], Martin Richter[1], Debkumar Rana[1], Ritesh Haldar[2], Christoph Wöll[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology, Germany

For the optimization of organic optoelectronic devices, it is important to understand the ultrafast electronically excited state dynamics in organic semiconductors after optical excitation. For instance, different molecular packing and relative orientations of the optically active chromophores can affect the excitonic coupling strength. This can be studied in crystalline molecular assemblies by integrating these chromophores into surface-mounted metal-organic frameworks (SURMOFs) as organic linkers. Varying the side-groups of the molecules enables to engineer the crystal structure to tune the excitonic coupling. To analyse the influence of this crystal engineering on the ultrafast dynamics we investigated thin films of chromophore functionalized Zn-SURMOF by means of femtosecond transient absorption.

CPP 49: Polymer and Molecular Dynamics, Friction and Rheology

Time: Friday 11:30–13:00 Location: H39

CPP 49.1 Fri 11:30 H39

Molecular Mobility and Physical Aging in Polymers of Intrinsic Microporosity (PIM-1) Revisited: A Big Glassy World — •Farnaz Emamverdi, Martin Böhning, and Andreas Schönhals — Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Polymers of Intrinsic Microporosity (PIMs) are promising candidates for the active layer in gas separation membranes because of their high permeability and reasonable permselectivity. However, PIMs suffer from a decrease in performance with time due to physical aging. The initial microporous structures approach a denser state via local rearrangements, leading to a reduction of the permeability. Hence a characterization of the molecular mobility in these materials can provide valuable information about physical aging. In this work, the dielectric behavior of PIM-1 films and their behavior upon heating (aging) were revisited during different heating/cooling cycles in a broad temperature range between 133 K and 523 K. In addition, the obtained results were compared with data of samples that were annealed at ambient temperatures for different time. Multiple dielectric processes were observed like different relaxations due to local fluctuations and a Maxwell-Wagner-Sillars polarization effects due to the microporosity. The temperature dependence of the rates of all the processes follows the Arrhenius law where the estimated activation energy depends on the process. The influence of the thermal history on the processes is discussed in detail.

CPP 49.2 Fri 11:45 H39

Orientation approach to the light-induced surface relief gratings formation in azopolymer materials — •Nina Tverdokhleb, Bharti Yadav, and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden e. V., PF 120411, 01005 Dresden

The phenomenon of azopolymer deformation giving rise to surface relief gratings (SRG) under the influence of polarized light was discovered two and a half decades ago. Despite the numerous different theoretical approaches to this effect, an accurate representation that would interpret all peculiarities of this phenomenon is absent. At present, the light-induced orientation of polymer backbones looks like the most promising explanation [1]. With help of this orientation approach and the finite element modeling software ANSYS, we simulate the viscoplastic formation of sinusoidal protrusions produced by the applied light-induced stress on the thin azopolymer films. We explain the difference in SRG height for irradiation with various interference patterns. It is found that the mechanical boundary conditions have a crucial impact on the output. The results of our viscoplastic modeling are in good agreement with recent experiments [2]. [1] B. Yadav et al. J. Phys. Chem. B 122 (2019) 2001-2009. [2] B. Yadav, N. Tverdokhleb et al. Macromol. Mater. Eng. (2022) 2100990.

CPP 49.3 Fri 12:00 H39

Measuring Volume Exclusion on Single Polymer Chains Diffusing in Solution — •Tobias Thalheim and Frank Cichos — Peter Debye Institute for Soft Matter Physics, Leipzig University, Germany

Excluded volume effects in single polymer chains occur due to long-range interactions of distant segments in the chain which cannot pass through each other entailing a strong influence of the static as well as the dynamic behavior of the polymer. Various theoretical descriptions were thus devised to incorporate these effects in the interpretation of experimental outcomes. A theory by Schäfer and Krüger incorporating this real-polymer phenomenon predicts a distribution function which describes the total segment density about an individual polymer's center of mass. This distribution function augments the picture of an ideal Gaussian chain by correction functions that account for volume exclusion and which were derived in the framework of renormalization groups. Although this permits the assessment of the role of volume exclusion for single chains in contrast to usual accesses via scaling theories or ensemble measurements, this theory has never been tested before. We report on experiments including two types of freely-diffusing double-stranded DNA molecules that utilize Schäfer's and Krüger's theory to investigate these effects. We show that for short λ-DNA molecules volume exclusion is of minor importance, whereas long T4-DNA molecules exhibit prominent volume exclusion. Furthermore, we employ a thermophoretic trapping method to test this theory on single compressed polymers subjected to a virtual harmonic potential.

CPP 49.4 Fri 12:15 H39

Dynamics in polymer-fullerene blends for photovoltaic applications studied with quasielastic neutron scattering — •Dominik M. Schwaiger[1], Wiebke Lohstroh[2], and Peter Müller-Buschbaum[1,2] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]MLZ, TU München, 85748 Garching

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed, 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 that is often used in combination with the fullerene derivate PCBM. 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, PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were performed 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 49.5 Fri 12:30 H39

Equilibration of free-standing films of highly entangled polymer melts — •Hsiao-Ping Hsu and Kurt Kremer — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128, Mainz, Germany

Equilibrating confined and free-standing films of highly entangled polymer melts is a challenge for computer simulations. We approach this problem by first studying polymer melts based on a soft-sphere coarse-grained model confined between two walls. The distance of the walls is compatible with the simulation box of bulk melts in equilibrium, while periodic boundary conditions in the directions parallel to the walls are kept. Then we successively insert more fine grained polymer representations until the underlying microscopic details of the bead-spring model are reached. Tuning the wall potential, the monomer density of confined polymer melts in equilibrium is kept at bulk melt density even near the walls. Switching to another recently developed variant of the bead-spring model we can study melts at zero pressure [1] and study free-standing polymer films [2]. Furthermore, this also allows us to study free-standing films under strain and analyze the influence of entanglements on the local film morphology.

[1] H.-P. Hsu, K. Kremer, J. Chem. Phys. 150, 091101 (2019); 150, 159902 (2019).

[2] H.-P. Hsu, K. Kremer, J. Chem. Phys. 153, 144902 (2020); 156, 019901 (2022).

CPP 49.6 Fri 12:45 H39

Liquid flow through nanoporous media: non-linear response and blocking — •Roya Ebrahimi Viand[1] and Felix Höfling[1,2] — [1]Department of Mathematics and Computer Science, Freie Universität Berlin, Germany — [2]Zuse Institute Berlin, Germany

Directed fluid flow is a major transport mechanism in porous media that can either be generated by pumps or emerge in response to a pressure gradient. The pressure-flow relation and how it depends on the structure and geometry of the medium is investigated by non-equilibrium molecular dynamics (NEMD) simulations of a flow of dense liquids through regular bead packings as a model for nanoporous medium. Upon decreasing the porosity, we find a significant non-linear response. The linear permeability varies over two orders of magnitude and vanishes beyond a critical porosity. Our simulations further exhibit a substantial increase in temperature inside the porous medium, which we attribute to the local balance of energy fluxes using fluid mechanical conservation laws. Finally, we show that a recent NEMD approach based on the adaptive resolution simulation (AdResS) technique can help to decrease the required simulation volume considerably [1,2]. This simulation approach is expected to be highly applicable for research on flow in porous as well as biological media.

[1] R. Ebrahimi Viand et al., J. Chem. Phys. 153, 101102 (2020)
[2] R. Klein, R. Ebrahimi Viand et al., Adv. Theory Simul. 4, 2100071 (2021)

CPP 50: Nanostructures, Nanostructuring and Nanosized Soft Matter

Time: Friday 12:30–13:00 Location: H38

CPP 50.1 Fri 12:30 H38

The effect of solvent vapor annealing on diblock copolymer templated mesoporous Si/Ge/C thin films — •Christian L. Weindl[1], Christian E. Fajman[2], Michael A. Giebel[2], Kerstin S. Wienhold[1], Shanshan Yin[1], Ting Tian[1], Christina Geiger[1], Lucas P. Kreuzer[5], Matthias Schwartzkopf[3], Stephan V. Roth[3,4], Thomas F. Fässler[2], and Peter Müller-Buschbaum[1,5] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]TU München, LS Anorganische Chemie mit Schwerpunkt Neue Materialien, Chemie-Department, 85748 Garching — [3]DESY, 22607 Hamburg — [4]Royal Institute of Technology KTH, 100 44 Stockholm — [5]MLZ, TU München, 85748 Garching

The latest research has revealed promising results for silicon (Si) and germanium (Ge) as anode materials for lithium-ion batteries. These two group 14 semiconductors are considered auspicious additives in graphite anodes due to their high specific capacity (Si) and electron mobility (Ge). This study aims to synthesize a mesoporous Si/Ge/C structure by using a wet chemical sol-gel approach with the structure-directing amphiphilic diblock copolymer PS-b-PEO and the Zintl cluster $K_{12}Si_xGe_{17-x}$. Furthermore, we investigate the structural changes on the spin-coated thin films upon exposure to a saturated toluene/butanol atmosphere. For morphlolgical analysis, scanning electron microscopy will be combined with grazing-incidence small-angle x-ray scattering (GISAXS). Moreover, energy-dispersive X-ray spectroscopy, Raman spectroscopy and powder X-ray diffraction are used for further elemental and crystalline phase analysis.

CPP 50.2 Fri 12:45 H38

The kinetics and free-energy landscape of grain-boundary motion incylinder-forming copolymers — •Niklas Blagojevic and Marcus Müller — Universität Göttingen, Institut für Theoretische Physik

Block copolymers which self-assemble into a dense array of hexagonally-packed cylinders are promising canditates for filtering membranes with pore sizes in the nanometer range used to extract or to purify a substance. The cylinders act as selective transport channels and it is important to align the cylinders along the desired flux direction. A fundamental understanding on how to control the cylinder orientation in the processing of the membrane, however, is incomplete and successful applications have often relied on trial-and-error searches in the high-dimensional space of process parameters.

To gain fundamental understanding about orientation mechanisms of cylindrical copolymer phases, we employ large-scale computer simulations of a particle based model in a highly efficient GPU-parallel implementation with sophisticated free-energy techniques. With this, we study the kinetics of grain-boundary motion of cylindrical copolymer domains – resembling the (re-)orientation mechanisms – and the Minimum Free-Energy Path of the associated changes of the domain topology. The simulation study has provided direct insights into the kinetics and the free-energy landscapes of orientation mechanisms and ordering in the early and late stages.

CPP 51: Overview Talk Claus M. Schneider (joint session O/CPP)

Time: Friday 13:15–14:00 Location: S054

Invited Talk CPP 51.1 Fri 13:15 S054

Exploring the Mysteries of Topology in Quantum Materials — •Claus M. Schneider — Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich

A characteristic feature of emergent or quantum materials is the competition of various spin-dependent interactions, such as spin-orbit coupling and exchange interaction. In addition, depending on the material system, there may be a breaking of time-reversal and/or inversion symmetries at play. As a consequence, topological materials may range from metals to insulators. In the vicinity of the Fermi level, this situation leads to peculiar electronic dispersions associated with Dirac and Weyl points, eventually also resulting in complex spin textures in momen- tum space. The interplay of competing mechanisms often results in unusual charge and spin transport phenomena in such materials. In order to understand the physical properties of quantum materials on a fundamental level, we need to explore these electronic states in detail and disentangle the role of the various interactions. For this purpose, we employ electron spectroscopic approaches, which explicitly take the electron spin as an experimental quantity into account. In this contribution we discuss an avenue starting from simple single-crystalline systems (e.g, W(011), Fe(100) and Co(100)) to more complex 2D and 3D quantum materials and detail the role of the individual interactions and symmetry-breaking mechanisms by experimental examples.