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 100×20 μm^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].

[1] A. Erbe, K.Tauer, R. Sigel, Phys. Rev. E 73, 031406 (2006)
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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.

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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 fine-tuned 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-HD}$_2$-T (PDPP$_T$) with thiophene flanking units and PDPP[T]$_2${2-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-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.

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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 University Jena, Humboldstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — [3]Institute of Chemical Biology, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, Athens 11635, Greece. — [4]Advent Technologies SA, Patras Science Park, Stadiou Street, Platani-Rio, 26504, Patra, Greece

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.

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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.

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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.

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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.

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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.

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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

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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.

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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.