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Poster abstracts

Postersession 1 (Sept. 26, 2024 / 17:30 – 20:00)

P1: A Lab-Based NAP-XPS Setup to Probe Photoelectrochemical Interfaces under Working Conditions

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Understanding complex (photo)electrochemical conversion processes at functional interfaces is closely linked to observations under operation. Our newly installed lab-based near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) setup from SPECS enables the study of heterogeneous interfaces under working conditions, providing rapid feedback during material development. The setup features three different monochromatic X-ray sources – Al K α (1487 eV), Ag L α (2984 eV), Cr K α (5415 eV) – allowing for probing depths of 2 - 20 nm to examine surfaces and buried interfaces. An ‘open-liquid’ three-electrode electrochemical cell enables operando measurements of solid|electrolyte interfaces. Additional external illumination allows us to examine photo-induced processes, such as photo(electro)catalytic and degradation processes, and the illuminated semiconductor|electrolyte interface. Experiments with this lab-based NAP-XPS system will contribute to the understanding of (photo)electrocatalyst behavior under operating conditions and fundamental chemical conversion processes at functional interfaces.

P2: ASYMMETRIC ACCEPTOR DESIGN WITH FUSED-IMIDAZOLE LINKAGES FOR EFFICIENT ORGANIC SOLAR CELLS

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In the pursuit of advancing organic solar cells (OSCs), the structural manipulation of non-fullerene electron acceptors (NFAs) plays a crucial role in enhancing device performance. This study presents BTQT-4F, a novel Y-series NFA with a fused-imidazole core, diverging from traditional pyrazine-based linkages. This five-membered-ring imidazole linkage enhances 3D charge transport and molecular packing. Femtosecond transient absorption (fs-TA) spectroscopy shows that BTQT-4F improves exciton dissociation and accelerates hole transfer, boosting charge transport. In a ternary blend with PM6 and BTP-eC9, BTQT-4F achieved a record power conversion efficiency (PCE) of 19.4%. This highlights the potential of fused-imidazole linkages in pushing the efficiency of organic solar cells.

[1] Liu, X et al *Angew. Chem., Int. Ed.* **2024**, 63, e202316039.

P3: BOUND- AND FREE EXCITON EMISSION IN I-III-VI QUANTUM DOTS

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Heavy metal free I-III-VI quantum dots (QDs) are of great interest in light emitting and energy harvesting applications due to their non-toxicity, tunable band gap and water solubility. The optical properties of these nanocrystals are usually determined by intrinsic defects, leading to

broad emission spectra. However, it has been shown that forming a core-shell structure of I-III-VI QDs can lead to the suppression of the broad defect related peak and an enhancement of free exciton emission. Here, we report two novel ways of synthesizing I-III-VI QDs. First, we show a simple and facile synthesis approach to produce QDs containing Ag, In and S with quantum yields exceeding 60% and comparably narrow defect related linewidth. Passivating the defect site with an inorganic shell, however, led to degradation of our QDs due to the high reaction temperature. Therefore, we report a second alternative synthesis procedure, which improves the stability of the QDs significantly. The optical spectrum indicates free exciton emission alongside a broad defect related emission peak. Forming a core-shell structure of these QDs with a high band gap inorganic material leads to pronounced luminescence of free excitons and the suppression of the defect emission.

P4: CHARGE TRANSPORT AND INTERFACIAL CHARACTERISTICS OF ALD CORROSION PROTECTION LAYERS ON SEMICONDUCTOR LIGHT ABSORBERS

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Producing value-added products via light-driven CO₂ reduction represents a promising approach to sustainably address increasing CO₂ emissions and meet the growing global energy demand. Such solar fuel systems require passivating layers to chemically protect semiconductor light absorbers from harsh reaction environments. Despite great progress in the development of atomic layer deposited (ALD) protection layers, the factors governing efficient charge injection into the catalytic component are not yet well understood. Here, the charge transport characteristics between various defect-engineered TiO₂ protection layers grown with ALD and metal catalyst layers are analyzed. Lateral transport characteristics are investigated using the transfer length method (TLM), aiming to provide insights into contact resistivity, carrier transport and interface kinetics within the protection layer.

P5: Dexter Energy Transfer from Quantum Dots to Closely-Bound Dye Molecules

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Quantum dots (QDs) are semiconductor nanocrystals confined in all three dimensions,^[1] whose optical properties can be systematically tuned by altering their size.^[2] By combining QDs with dyes, we can make hybrid QD-dye systems that exhibit efficient energy transfer (ET) from QDs to dyes, important for sensing and lighting applications. ET usually proceeds through Förster resonance energy transfer (FRET) that requires significant spectral overlap between QD emission and dye absorbance, and large oscillator strengths of those transitions. This severely limits the choice of suitable dyes. Perovskite QDs do not require passivating inorganic shells for bright emission, which makes ET mechanisms beyond FRET accessible. This work explores the design of a CsPbBr₃ QD-dye system to achieve efficient ET from CsPbBr₃ QDs to dyes with dimethyl iminium binding groups, where the close binding of dyes to the CsPbBr₃ surface should

facilitate spatial wavefunction overlap. We observe efficient ET from CsPbBr₃ to dyes with minimal spectral overlap. We show by steady-state and time-resolved photoluminescence experiments that the ET proceeds via the Dexter exchange-type mechanism. This significantly improves the tuneability of such QD-dye systems. This approach opens new avenues for QD-molecule hybrids for a wide range of applications, such as lighting.^[3]

[1] A. Barfüßer, S. Rieger, A. Dey, A. Tosun, Q. A. Akermann, T. Debnath, J. Feldmann. *Nano Lett.*, 22, 8810–8817 (2022)

[2] Q. A. Akkerman, T. P. T. Nguyen, S. C. Boehme, F. Montanarella, D. N. Dirin, P. Wechsler, F. Beiglböck, G. Raino, R. Erni, C. Katan, J. Even, M. V. Kovalenko. *Science* 377, 1406–1412 (2022)

[3] M. Kurashvili, J. Llusar, T. Würthner, D. Ederle, I. Infante, J. Feldmann, Q. A. Akkerman. (Manuscript submitted for publication)

P6: Effects of rotatable groups on metal organic frameworks

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Metal organic frameworks (MOFs) have found a number of successful applications, for example as gas storage or as filters for gas mixtures. So far, in those applications they have only been used as passive materials but recent research shows that their susceptibility to electric fields can be used to adjust their filter properties [1]. Current research tries to go a step further and incorporates rotatable linker groups within the framework to manipulate their rotation statistics using electric fields [2]. That way, for example, nano-pumps could be created which in turn could massively improve the filter properties of the MOF or enhance the MOF's storage capabilities by using these linkers as adjustable "doors". In our research we use density functional theory (DFT) and Monte-Carlo simulations to sample rotational energy barriers and dipole moments to understand ion movements and ferroelectric effects inside MOFs to rate their capacity as nano-rotors.

[1] *Defibrillation of soft porous metal-organic frameworks with electric fields*, A. Knebel et al, *Science*. 358, 347–351 (2017).

[2] *Coordination Networks: Building Blocks for Functional Systems*, H. Oberhofer, D. Volkmer, A. Wixforth, DFG Proposal. DFG priority programme 1928 (COORNETs), Granting period II (2020 – 2022) (2018).

P7: Excited state dynamics and performance optimization of diketopyrrolopyrrole-based DSSCs for solar energy conversion

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Three diketopyrrolopyrrole-based dyes were incorporated into DSSCs, featuring a layer of TiO₂ nanoparticles as semiconductor, iodide/triiodide redox electrolyte, and a platinum counter electrode. Optimization of these devices with respect to I₂ and Li⁺ concentration of the electrolyte and the thickness of the TiO₂ layer revealed an optimum concentration of 0.1 M for both I₂ and Li⁺. Interestingly, the optimal layer thickness varied between the different dyes. All samples were characterized in depth on the basis of J-V assays, IPCE, and electrochemical impedance spectroscopy. Furthermore, fs- and ns- transient absorption spectroscopy for TiO₂-based and Al₂O₃-based cells provided fundamental insights into the DSSC excited state dynamics.

P8: EXTRACTION OF HOT CARRIERS IN COLLOIDAL CSPBBR₃ NANOCRYSTALS

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Extraction of hot charge carriers holds great promise for enhancing the solar energy conversion efficiency.^[1] This study investigates the role of capping ligands in colloidal perovskites in facilitating the extraction of photogenerated hot electrons. By integrating colloidal CsPbBr₃ with fullerene-based capping ligands, we achieve efficient electron transfer with near-unity fluorescence quenching. The detailed hot carrier dynamics is studied by ultrafast transient absorption (TA) spectroscopy together with global analysis. Moreover, hot carrier cooling processes have been derived from the fitting of the high-energy tail of photoinduced bleach in TA spectra. We demonstrate the presence of fullerene ligands results in a three-fold increase in the relaxation time of hot carriers and a significant hot carrier extraction efficiency of 65.6%. This work underscores the potential of engineering surface ligands of colloidal perovskites to boost hot carrier extraction.

[1] Li, M et al *Nat. Commun.* **2017**, *8*, 14350.

P9: First-principles study of phenolic anchor groups for molecular water oxidation catalysts on modified WO₃ surfaces

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WO₃ is a promising anode material for photocatalytic water splitting, but its efficiency is limited in particular by the oxygen evolution reaction. In collaboration with experiment we aim to increase this efficiency by attaching catalytically active complexes to WO₃ surfaces. The complexes must bind to the surface and should electronically couple to it. Here we investigate using first-principles simulations whether phenol, catechol, resorcinol and hydroquinol could theoretically be considered as anchor groups. We created a hydroxylated (001) WO₃ surface model and used it to study different binding modes of the ligands based on PBE-D3-DFT geometry optimizations. The results indicate that for all ligands, covalent binding is energetically unfavorable compared to water adsorption and dispersive anchoring is in clear competition with surrounding water molecules. For the latter adsorption mode, real-time-real-space TDDFT confirms that no strong electronic coupling is to be expected.

We acknowledge discussion with G. Hörner, University of Jena, Anorganic Chemistry III, and R. Marschall, University of Bayreuth, Physical Chemistry III.

P15: INFLUENCE OF TEMPERATURE AND LIGHT ON THE STRUCTURE OF LEAD HALIDE PEROVSKITE NANOCRYSTALS

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Perovskite nanocrystals are very promising in contributing to the renewable energy mix of the future by being used as an active layer within photovoltaics. They are comparable stable to bulk perovskite solar cells, and provide high power conversion efficiencies and a high photoluminescence quantum yield. Furthermore, the range of usable X halides (I⁻, Br⁻, Cl⁻) and A cations (FA⁺, MA⁺, Cs⁺) enables fine control of the bandgap over the whole visible spectrum

of the ABX₃ perovskite structure.

In this work, cesium lead iodide (CsPbI) and formamidinium lead iodide (FAPbI) nanocrystals have been mixed in different ratios and deposited via slot-die coating. These perovskite nanocrystals as active layers are investigated using grazing-incidence wide-angle X-ray scattering (GIWAXS) to reveal their crystal structure and texture during temperature changes and permanent illumination.

P11: Guest-Mediated Modulation of Photophysical Pathways in a Coronene Bisimide Cyclophane

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The properties and functions of chromophores utilized by nature are strongly affected by the environment formed by the structure in the cells surrounding them. This concept is transferred here to host-guest complexes with the encapsulated guests acting as environmental stimulus. A new cyclophane host based on coronene bisimide is presented that can encapsulate a wide variety of planar guest molecules with binding constants up to $4.29 \times 10^{10} \text{ M}^{-1}$ in chloroform. Depending on the properties of the chosen guest, the host-guest complexes can be tuned towards fluorescence, exciplex formation, charge separation, room temperature phosphorescence or thermally activated delayed fluorescence. The photophysical processes were investigated by absorption, emission, femto- and nanosecond transient absorption spectroscopy.

[1] J. R  he, K. Vinod, H. Hoh, K. Vinod, K. Shoyama, M. Hariharan, F. W  rthner, *J. Am. Chem. Soc.*, 2024, *accepted manuscript*.

P12: HIGH-PRESSURE METHODOLOGY FOR CLARIFYING PCET MECHANISMS IN GROUND AND EXCITED STATES

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We have elucidated the mechanism of excited-state proton-coupled electron transfer (PCET) for a model reaction, as depicted in Scheme 1 [1], using pressure-dependent measurements obtained through femtosecond and nanosecond resolved transient absorption spectroscopy (TAS) with a custom-built high-pressure detection cell. This unique study of excited-state PCET under high-pressure conditions has allowed us to demonstrate the effectiveness of variable pressure measurements in excited-state chemistry. Specifically, we were able to differentiate between stepwise and concerted PCET processes and introduce the concept of using pressure to modulate PCET mechanisms. This talk will also illustrate how our pressure-based approach can be broadly applied to PCET processes, including ground-state reactions, by employing techniques such as high-pressure NMR or stopped-flow methods.

[1] A. Pannwitz, O.S. Wenger, *Phys. Chem. Chem. Phys.*, 18, 11374 (2016).

P13: Homoleptic Complexes of Bis(4-carboxypyrazol-1-yl)acetic acid: a New Building Unit for MOFs

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Bis(4-carboxypyrazol-1-yl)acetic acid (H3bcpza) ligands show new possibilities in coordination behavior due to the additional peripheral carboxylic acid groups on the pyrazoles [1]. The coordination behavior of H3bcpza was explored upon synthesis of several homoleptic transition metal complexes [M(L)2]. These homoleptic complexes [M(L)2] show potential as building units for new metal-organic frameworks (MOFs). The single crystal structure analysis revealed that such microporous materials of the composition [M3(bcpza)2]_n × 12 H₂O (M = Cu) exhibit a highly regular structure comprised from essentially two building units: the homoleptic units {M(bcpza)₂} and paddle-wheel moieties {M₂(CO₂)₄}. The MOF was studied by powder XRD, TGA and BET analyses. According to the data the MOF might be suitable for solar driven atmospheric water harvesting (AWH). Current work focuses on a spacer between the pyrazole and carboxylate moieties in order to vary the pore size of the MOFs.

[1] W. Tzegai et al, *Dalton Trans.* 51. 6839 (2022).

P14: Influence of Carbonyl Functionalization in a Molecular Cleft on O-O Bond Formation Mechanism in Light-Driven Water Oxidation

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A series of carbazole derivatives incorporated in a Ru(bda) based synthetic molecular cleft (bda = 2,2'-bipyridine-6,6'-dicarboxylate) for light-driven water oxidation catalysis were synthesized. Three different substituents at the carbazole nitrogen atom were employed: a carboxylic acid, a methyl ester, and a primary amide. Photocatalytic measurements at neutral pH revealed distinct mechanistic pathways for these derivatives. The carboxylic acid derivative **C1** exhibits a unimolecular water nucleophilic attack (WNA) mechanism, whereas the methyl ester **C2** and primary amide **C3** operate via a less efficient intermolecular coupling of two metal-oxo species (I2M). Single crystal X-ray analysis of **C1** provided structural insights, revealing an intramolecular hydrogen bond between the acidic proton of the carboxylic acid moiety and an oxygen atom of the Ru(bda) unit. This intramolecular interaction presumably keeps the catalytic ruthenium centre in the cavity during catalysis, thereby facilitating the preferred WNA mechanism. The study highlights the potential of molecular design in tuning catalytic activity and efficiency, offering valuable insights for the development of more effective water oxidation catalysts.

P15: Giant rare-earth catecholate crystals- morphology control and rapid NIR luminescence response

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Lanthanide coordination polymers (Ln-CPs) have attracted significant interest as near-infrared (NIR) emitting materials. In this study, we elucidate the rapid NIR response of two catecholate-based coordination polymers, specifically Yb-DHBQ and Nd-DHBQ (DHBQ = 2,5-dihydroxy-1,4-benzoquinone). In addition, through controlled crystallization we have isolated two structural variances of Yb-DHBQ. Moreover, by optimizing the reaction conditions, we achieved

precise control over the crystal morphology, extending their size up to 500 μm .

P16: INTRAMOLECULAR DOWN- AND UP-CONVERSION IN DIMERIC TETRACENE COMPLEXES CENTERED VIA PLATINUM(II) AND PALLADIUM(II)

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Singlet fission (SF), also called down-conversion, and triplet fusion, also called triplet-triplet annihilation up-conversion (TTA-UC) are reversed multiexcitonic processes. They have the potential to increase solar energy conversion efficiencies beyond current limitations.^[1-3] In tetracene, where the energy of singlet exciton is nearly twice the energy of triplet exciton. As such, both SF and TTA-UC are thermodynamically feasible.^[3] In this project, we design and synthesize Pt(II) and Pd(II) centered tetracene dimer complexes using pyridyl-encapped tetracene ligand via a one-pot protocol. Notably, for the Pt(II)-coordinated tetracene dimer, intramolecular down- and up-conversion processes are facilitated despite the large distance between the tetracene chromophores. It demonstrates that the metal center plays a crucial role in controlling the excited state reactivity of tetracenes.

[1] Smith, M. B. & Michl, J. *Chem. Rev.* **110**, 6891–6936 (2010).

[2] Shockley, W. & Queisser, H. J. *J. Appl. Phys.* **32**, 510–519 (1961).

[3] Singh-Rachford, T. N. & Castellano, F. N. *Coord. Chem. Rev.* **254**, 2560–2573 (2010).

[4] Bo, Y. et al. *J. Am. Chem. Soc.* **145**, 18260–18275 (2023).

P17: Investigating the iodoplumbate complex evolution of perovskite solution during spin coating via UV-VIS in-situ spectroscopy

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The solution-based fabrication of reproducible, high-quality metal halide perovskite films demands a detailed understanding of the film formation, particularly with regard to the crystallization dynamics. Since perovskite crystals form from solution, it is the perovskite precursor solution and its processing conditions that determine the final structure and morphology of the perovskite film. The precursor chemistry in stock solution has been widely investigated. However, the role of the precursors in film formation remains a topic of discussion. Therefore, we conduct a systematic in situ study during the critical phase before the nucleation. Using UV-VIS absorption spectroscopy during spin coating (i.e. in situ) allows us to track the evolution of iodoplumbate complexes present in the precursor solution. We find that a novel absorption signature arises and attribute this to the emergence of a crystalline PbI₂-DMF solvated (PDS) phase during spin coating. The amount of PDS phase is closely connected to the concentration of the precursor solution film, which we estimate using white light interference. We also propose that PDS crystallites are a predecessor of crystalline perovskite phases and act as nucleation seeds in the precursor solution.

P18: INVESTIGATIONS ON THE OPTOELECTRONIC PROPERTIES OF COMPOUNDS BEARING SMALL HOMOATOMIC CLUSTERS OF THE TETREL ELEMENTS

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The *Zintl* phases of type A₄E₄ and A₄E₉ feature small homoatomic four- and nine-atom clusters of the semiconducting elements silicon and germanium. Even through these compounds have

been known for decades, only few investigations of their optoelectronic properties have been reported. [1,2,3] Herein we present a first study of A_4E_4 ($A = \text{Na, K, Rb, Cs}$; $E = \text{Si, Ge}$) and $A_4\text{Ge}_9$ ($A = \text{K, Rb, Cs}$) on optical band gaps determined *via* diffuse reflectance spectroscopy and the electronic properties obtained by quantum chemical methods. Furthermore, we compare the results found for $A_4\text{Ge}_9$ with them for compounds in which $A_4\text{Ge}_9$ co-crystallizes with $A_3[\text{MO}_4]$ ($M = \text{transition metal}$) forming double-salts of the composition $A_{11}[\text{Ge}_9]_2[\text{MO}_4]$ and discuss the exceptional stability of the *Zintl* anion towards the $[\text{MO}_4]$ unit, as well as possible charge transfers between the building units in these hybrid materials.

[1] Imai Y., A. Watanabe A., *J. Alloys Compd.* 478, 754-757 (2009). [2] Tegze M., Hafner J., *Phys. Rev. B*, 40 (14), 9841-9845 (1989). [3] Imai M., Yamada T., et al., *Jpn. J. Appl. Phys.*, 61, 031004|1-5 (2022). [4] Fässler T. F. et al, *Angew. Chem. Int. Ed.*, 51, 742-747 (2012). [5] Fässler T. F., et al., *Inorg. Chem.*, 51, 4058-4065 (2012).

P19: LANGMUIR-BLODGETT PREPARED P-N-JUNCTION POLYMER FILMS AS A PLANAR HETEROJUNCTION IN ORGANIC-BASED SOLAR CELLS

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Advances in solution processing techniques have enabled the creation of electronic devices using organic thin films [1,2]. The current simple yet effective layer-by-layer organic solar cells are commonly prepared using the blade- or spin-coating. An alternative solution-based method is the Langmuir-Blodgett (LB) technique, which offers fabrication of films with a monolayer-precision on the nanometer range. We report on the successful use of p-n junction polymer composite of superior structural quality fabricated via LB for application in organic-based solar cells. The polymer blend composite consists of PM6 donor and N2200 acceptor materials, both known for high OPV device performance. Our multi-step fabrication of the layers resulted in thickness of 7 nm for each polymer, allowing maximum exciton dissociation and preventing exciton quenching before diffusing into donor/acceptor interface [3].

[1] K. Gubanov et al, *Adv. Electron. Mater.*, 9, 2201233 (2023).
[2] T. Hawly et al, *ACS Appl. Electron. Mater.*, 4, 5914 (2022).
[3] C. J. Brabec et al, *Adv. Mater.*, 22, 3839–3856 (2010).

P20: Learning an effective hamiltonian of temperature-dependent electronic structure using machine learning

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Calculating the optoelectronic properties of large-scale systems across varying temperatures using standard density functional theory (DFT) can present significant computational challenges. By leveraging machine learning force fields (ML-FFs), it has become easier to generate trajectories at different temperatures. Nonetheless, obtaining the temperature-dependent electronic structure remains a complex task. Building on our prior research involving a model for an effective Hamiltonian in a localized basis [1], we propose a method that integrates ML techniques to increase the accuracy and computational efficiency of the approach. The synergy of ML and effective Hamiltonian models has the potential to facilitate the exploration of material properties across different temperatures with reduced computational demands and perform multiscale and high throughput calculations with high efficiency.

[1] M. Schwade, M.J. Schilcher, C. Reverón Baecker, M. Grumet, D.A. Egger, *J. Chem. Phys.* 160, 134102 (2024).

P21: Mechanistic Investigations of the Disulfide Activation Process

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P22: Mechanistic Investigations of the Disulfide Activation Process

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A detailed investigation of the activation of disulfide molecules for biocompatible disulfide-ene reactions is shown.[1] The photocatalyzed triplet-triplet energy transfer was followed by means of steady-state and transient spectroscopy. The focus of investigations lies on the influence of the sterical hindrance of the disulfide substituents on the triplet-triplet energy transfer. The results were corroborated by theoretical calculations.

[1] Teders, M., Henkel, C., Anhäuser, L. et al. The energy-transfer-enabled biocompatible disulfide-ene reaction. *Nature Chem* **10**, 981–988 (2018). <https://doi.org/10.1038/s41557-018-0102-z>

P23: Mapping the photocatalytic reactive sites of 2D materials

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Photocatalysts have attracted significant interest due to their ability to facilitate chemical production under mild conditions through light-matter interactions [1]. Extensive research highlighted the importance of studying the interactions between molecules and nanomaterials to uncover and comprehend the broad applicability of photocatalysis. To date, the scanning electrochemical microscope (SECM) is the sole technique capable of locally studying chemical production from purely photocatalytic processes and enabling the precise mapping of these produced chemicals [2].

Here, we present a methodology using SECM to spatially identify the photo-active sites in 2D materials, allowing quantitative mapping of the generated products. We evidenced the clear spatial separation of photocatalytic reactive sites, which were associated to the light spot location. By combining experimental results with a diffusion model, we quantified the quantum efficiency of photocatalysts [3]. This approach can ultimately be used to explore the relationship between system properties and the photoproducts.

[1] M. Melchionna, P. Fornasiero, *ACS Catal.* (2020), **10** (10), 5493–5501

[2] N. Casillas, P. James, W. H. Smyrl, *Journal of the Electrochemical Society* (1995), **142** (1), L16-L18

[3] O. Henrotte et al., *ACS Nano* (2023), **17** (12), 11427-11438

P24: MULTISTATE PHOTOSWITCHES BASED ON NEARLY PANCHROMATIC NORBORNADIENE-TRIAZINE HYBRID STRUCTURES AS POTENTIAL DATA STORAGE SYSTEMS

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A very efficient and well-investigated photoswitch system is the norbornadiene/ quadricyclane (NBD/QC) interconversion couple. Besides usage as so called molecular solar thermal (MOST) fuels,^[1] implementation in potential data storage systems or as logical gates, like i.e. as keypad lock was considered recently.^[2] Through precise structural modifications of the parent carbon scaffold, a change of the related photophysical properties can be achieved. By attaching multiple photoswitches to a single core, individually switchable units resulting in different accessible states are obtained. The investigated molecules are synthesized starting from a triazine moiety as central acceptor with different electron donating groups attached on the NBD to tune the absorption properties and thus enable individual switching. By irradiating into the respective absorption bands, and reversible protonation of an amine functionality, a total of 8 different states can theoretically be accessed.

[1] Z. Wang et al., *Joule* **2021**, 5, 3116–3136.

[2] A. Dreos et al., *J. Phys. Chem. Lett.* **2018**, 9, 6174–6178.

P25: Overcoming Optical Losses in Thin Metal-Based Recombination Layers for Efficient n-i-p Perovskite-Organic Tandem Solar Cells

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Perovskite-organic tandem solar cells (P-O-TSCs) show the potential to exceed single-junction efficiency limits. However, their performance is hampered by non-ideal interconnection layers (ICLs). Metal nanoparticles are conventionally incorporated into ICLs to facilitate effective carrier recombination, yet negatively introduce serious parasitic absorption, particularly in the near-infrared region. Thus, alleviated photon utilization in the organic rear cell decisively constrains the maximum photocurrent matching with the front cell. Here we report a novel strategy to reduce this optical loss in the Au-embedded ICLs by tailoring the shape and size distribution of Au nanoparticles via manipulating the surface property of the underlying layer. Smaller and more regular spherical Au nanoparticles show significantly reduced optical losses due to a reduced localized surface plasmon resonance in the spectral regime of the organic rear cell while still providing efficient recombination pathways. Consequently, optimized P-O-TSCs combining CsPbI₂Br with various organic cells benefit from a substantial current rise of >1.5 mA/cm² in the organic rear cells. Meanwhile, P-O-TSCs with optimized ICLs demonstrate promising long-term device stability.

P26: Plasmonic-induced Thermoelectric Effects in Polymer Electrolytes

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The ability to generate local heat by the energy dissipation of photoexcited surface plasmon resonances in metal nanoparticles (NPs) has attracted manifold interests, leading to first applications in photothermal cancer therapy or devices for energy conversion. We utilize this effect in an all-transparent polymer electrolyte device to create an additional temperature

gradient (TG) by the selective light absorption. Due to the ion conductivity of the electrolyte this results in a remarkable thermovoltage via the Soret effect. Our device, optimized for resonant excitation at 532 nm, features a 2D array of Ag nanotriangles bedded in a PEGMA /BEMA polymer blend with LiTFSI as conducting salt [1]. The TG generated by the excited plasmonic NPs is significantly higher than for a non-plasmonic reference, resulting in a maximum thermovoltage of 101 mV at 4 mW excitation. By comparing different geometries we will highlight the relevant photophysical processes leading to the observed thermoelectric effects.

[1] M. Frank, J. Pflaum, *Adv. Funct. Mater.* **2022**, *32*, 2203277.

P27: PREPARATION AND ISOLATION OF P3HT SUPERSTRUCTURES WITH DIRECTED ENERGY GRADIENTS

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The precise funneling of excitation energy toward the reaction centers is a key step in photosynthesis, which is often established using a single type of pigment molecules. Typically, artificial approaches realize energy funnels by relying on energy transfer cascades along many chemically different molecules. Here, we demonstrate an elegant concept based on supramolecular objects for the efficient nucleation of the conjugated polymer poly(3-hexylthiophene), P3HT [1], which allows us to prepare, isolate, and study tailored superstructures. We show that the aligned P3HT nanofibers in the superstructures feature a directed energy gradient over micrometer distances.[2]

[1] F. A. Wenzel et al, *Macromolecules*. *55*, 2861–2871 (2022).

[2] S. Stäter et al, *Journal of the American Chemical Society*. *145*, 13780–13787 (2023).

P28:RANDOM LASING IN FLUORESCENT SILICA AEROGELS: FROM RHODAMINE 6G TO CARBON DOT DOPED COMPOSITES

Anithadevi Sekar, Matthias F Kestler, Theobald Lohmüller, Jochen Feldmann

Ludwig Maximilian University of Munich, Germany

Silica aerogels, known for their extremely low density, high surface area, and excellent light-scattering properties, are highly suitable materials for various optical applications, including random lasing. Here, we describe the synthesis of fluorescent silica aerogels through the supercritical drying of liquid gels doped with fluorescent dyes or carbon dots. Our optimized process produces an amorphous, porous network of colloidal particles, where scattering events result in closed photon paths that act as micrometer-scale cavities. We examine the photoluminescence, amplified stimulated emission, and random lasing spectra of various dye-loaded aerogel samples. Notably, the low thermal conductivity of aerogels leads to high thermal stability, enabling high laser pumping energies without visible sample degradation.

P29: Revealing Degradation Mechanisms in 2D/3D Perovskite Solar Cells under Photothermal Accelerated Aging

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Two-dimensional/three-dimensional (2D/3D) heterojunctions in perovskite solar cells exhibit

excellent optoelectronic properties and enhanced stability under mild aging conditions. However, their performance degrades drastically under harsh aging conditions. This study reveals the intrinsic instability of Ruddlesden-Popper (RP) perovskites under photo-thermal aging, which decompose into PbI_2 and metallic lead (Pb^0). The structural collapse promotes vacancy formation and facilitates iodide migration to the anode. Compared to RP/3D, Dion-Jacobson (DJ)/3D interfaces demonstrate superior structural stability and effectively block iodide migration into the transporting layer. However, blocking-induced uneven iodide distribution leads to interstitial defect formation in the 3D layer, exacerbating non-radiative recombination. To address it, we propose a strategical method by incorporating DJ in the 3D bulk instead of on the top surface, which effectively confines mobile ions within the grain and suppresses cation phase segregation. This optimization yields stable perovskite solar cells with an extrapolated operational T_{80} lifetime exceeding 560 hours under harsh conditions (85°C and 2-sun illumination).

P30: Self-Assembly of Nitrogen-Doped Helical Aromatic Bisimides into J-Aggregates

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Julius-Maximilians Universität Würzburg, Germany

Ever since their discovery in the late 1930s, J-aggregates have fascinated scientists because of the unique properties that result from their supramolecular structures. In particular, the desirable optical properties of a narrowed, bathochromically shifted absorption band with near-resonant fluorescence and an enhanced radiative rate accompanied by the ability to transport energy by exciton migration over large distances are of great interest for potential applications in functional materials. [1] In this work, we present the synthesis and characterization of a new nitrogen-doped helical aromatic bisimide (HBI) dye and J-aggregates thereof that are readily accessible via a cascade reaction. [2] Compared to previous work on perylene bisimide (PBI) based J-aggregates, the new hydrogen-bonding motif and the contorted [4]helicene backbone of the HBI chromophore facilitate the self-assembly into creeper helical J-aggregates. Detailed investigations of the self-assembly process and the resultant optical properties are correlated with structural insights into this new helical J-aggregate to elucidate the intriguing features of the HBI system.

[1] M. Hecht, F. Würthner, *Acc. Chem. Res.* 54, 642–653 (2021).

[2] X. Tian, K. Shoyama, F. Würthner, *Chem. Sci.* 14, 284–290 (2023).

P31: Structural Analysis of Lead Halide Perovskites

Lukas Max Rescher, Bert Nickel

Ludwig-Maximilians Universität München, Germany

We are interested in the structure of lead halide perovskite (LHP) films, especially those with large organic cations (LOC). We find that LOCs favour the formation of phases which deviate from the well known 3D structure. Our special interest is to find out if the crystallization and orientation of these phases can be influenced by processing steps during spin coating. These grazing incidence WAXS experiments are performed in collaboration with the group of M. Kaltenbrunner (JKU Linz). [1] In the case of colloidal nanoparticles, we are interested in the spontaneous halide exchange in solutions (Br to Cl and vice versa). We track probe this exchange via lattice constant changes observed by in-situ WAXS, and by small angle scattering experiments. We compare the lattice constant change with optical spectroscopy data from Q. Akkerman (LMU Munich). [2]

[1] L. E. Lehner et al, *Advanced Materials*, <https://doi.org/10.1002/adma.202208061> (2022)

[2] A. Akkerman et al, *Journal of the American Chemical Society*, <https://doi.org/10.1021/jacs.5b05602> (2015)

P32: Supramolecular Porphyrin-Perylenebisimide Bola-Amphiphiles

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¹Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; ²GW4 Facility for High-Resolution Electron Cryo-Microscopy, University of Bristol, Bristol, UK

The formation of stable hydrogen bonding motifs in water is challenging, due to the ubiquitous competition with the water molecules themselves. Nature circumvents this in e.g. DNA base pairs by shielding the motifs in hydrophobic pockets.[1] Transferring this concept to artificial light-harvesting systems, we envisioned a hierarchical, self-assembling perylenebisimide (PBI) – porphyrin bola-amphiphile, connected *via* hydrogen bonds. Using an amphiphilic cyanuric acid porphyrin, and a Hamilton receptor PBI, we studied the stabilization of this motif in a liposome superstructure.

[1] T. Sawada, M. Fujita, *J. Am. Chem. Soc.* **2010**, 132, 7194–7201.

P33: SYNTHESIS AND CHARACTERIZATION OF CHIRAL ORGANOBORON FOR BIOIMAGE APPLICATIONS

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Fluorophores are essential for imaging cells, tissues, and living organisms, significantly advancing biological and biomedical research. Ideal fluorophores must possess several key qualities, including long absorption and emission wavelength, large Stokes shifts, high brightness and stability.[1-4] Although many commercially available and known fluorophores have high molar extinction coefficients and strong fluorescence quantum yields suitable for bioimaging, they often suffer from small Stokes shifts. This limitation leads to poor signal-to-noise ratios and self-quenching in advanced imaging techniques.[2-4] Additionally, small Stokes shifts restrict their use in complex imaging methods, such as single-excitation multicolor imaging.[2] To overcome this limitation, we have developed and synthesized novel chiral boron complexes based on azinylcarbazoles[3,4] and azabora[7]helicene substructures,[5] starting from carbazole.

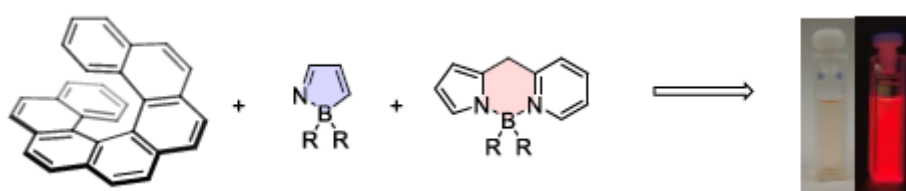


Figure 1: The design of novel chiral boron complexes with NIR emission.

In this poster, we report on the photophysical studies (absorption and emission spectra, CD measurements) and electrochemical properties (cyclic voltammetry) of these new compounds.

[1] G. Jiang, H. Liu, H. Liu, G. Ke, T.-B. Ren, B. Xiong, X.-B. Zhang, L. Yuan, *Angew. Chem. Int. Ed.* **63**, e202315217 (2024).

[2] H. Liu, G. Jiang, G. Ke, T.-B. Ren, L. Yuan, *ChemPhotoChem.* **8**, e202300277 (2024).

[3] K. Yamamoto, S. Matsui, S. Kato and Y. Nakamura, *Org. Biomol. Chem.* **21**, 5398–5405 (2023)

[4] M. Mas-Montoya, M. F. Montenegro, A. E. Ferao, A. Tarraga, J. N. Rodríguez-Lopez, D. Curiel, *Org. Lett.* **22**, 3356–3360 (2020).

[5] J. Full, S. P. Panchal, J. Götz, A.-M. Krause, A. Nowak-Król, *Angew. Chem. Int. Ed.* **60**, 4350-4357 (2021).

P32: Theoretical determination of tungsten trioxide clusters for photocatalytic water splitting

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Tungsten Trioxide (WO₃) is attractive as a photoanode for photocatalytic water splitting as it absorbs light and is stable in acidic conditions. In a joint experimental and theoretical effort [1] we plan to investigate the rate limiting step in photoelectrochemical water splitting, which is the oxidation of water. To this end, mesoporous photoanodes built from WO₃ particles are going to be realized. In order to gain a more profound understanding of such systems, we investigated the geometrical and electronic structure of WO₃ particles and their surfaces. A systematic construction rule has been developed to set up educated guesses for WO₃ clusters of considerable size including local bulk features. Furthermore, we study how geometrical and electronic properties of WO₃ clusters develop with increasing size and compare them to the WO₃ monoclinic crystal. Using ab-initio Born-Oppenheimer molecular dynamics we searched for further stable configurations for specific WO₃ systems.

[1] Collaboration with the groups of R. Marschall and B. Weber, University of Bayreuth

P34: ULTRAFast DYNAMICS OF A MEROCYANINE DYE-BASED ARTIFICIAL LIGHT-HARVESTING ANTENNA

Rebecca Fröhlich¹, Ajay Jayachandran¹, Alexander Schulz², Franziska Schneider², Matthias Stolte³, Frank Würthner^{2,3}, Tobias Brixner^{1,3}

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We use transient absorption and coherent two-dimensional electronic spectroscopy to investigate the exciton dynamics in an artificial light-harvesting antenna consisting of four dipolar merocyanine dyes [1]. The excited-state lifetime depends on the folding degree of the heteromer structure which is tunable by its solvent environment. With global analysis we follow the efficient ultrafast energy transfer between the chromophores and the localization of the excitation energy on the lowest exciton state in solvents of different polarity.

[1] A. Schulz et al, Chem (2024), <https://doi.org/10.1016/j.chempr.2024.05.023>.

P35: Unraveling the chirality transfer from circularly polarized light to single plasmonic nanoparticles

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Recently, chiral plasmonic nanostructures have drawn great interest due to their unique chiroptical properties [1]. Here, we thoroughly investigate the plasmon-assisted growth of chiral nanoparticles from achiral Au nanocubes (AuNCs) via circularly polarized light (CPL) without any chiral molecules. We identify the structural chirality of our synthesized chiral plasmonic nanostructures by using circular differential scattering (CDS) spectroscopy correlated with scanning electron microscopy imaging at both the single-particle and ensemble levels.

Theoretical simulations reveal that the plasmon-induced chirality transfer is mediated by the asymmetric distribution of hot electrons on achiral AuNCs under CPL excitation. Results presented here reveal fundamental aspects of chiral light-matter interaction, influencing the future design and optimization of chiral sensors and chiral catalysis, among others.

[1] R. M. Kim et al, *Nature*. 612., 470–476 (2022).

P36: Real-space transport channels in halide perovskites

Frederik Vonhoff, Maximilian J. Schilcher, David A. Egger
Technical University of Munich, Germany

For the progression towards commercialization of efficient solar cells based on halide perovskites, an understanding of the charge transport is needed. However, the theoretical descriptions of their transport properties require complex models and sophisticated methods due to their anharmonic atomic dynamics, resulting in an unusual transport behavior [1]. Here, we model the mobilities of MAPbI₃ and MAPbBr₃ via a time-dependent real-space model parametrized with hybrid density functional theory, incorporating anharmonicity via molecular dynamics trajectories. We analyze the influence of signatures in the band structure on electron and hole transport, focusing in particular on the projected density of states and the halide orbital contributions. Finally, we provide an intuitive real-space transport picture consisting of three transport channels, each driven by one of the three hopping interactions present in these materials.

[1] M. J. Schilcher et al, *Phys. Rev. Mater.* 7, L081601 (2023).

Postersession 2 (Sept. 27, 2024 / 10:15 – 11:45)

P1: Advancing photosystem II-based electrodes for photoelectric conversion

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Natural photosynthesis through photosystem II (PSII) efficiently converts solar energy, surpassing synthetic catalysts in water oxidation.[1-2] To harness this for sustainable energy conversion, we have immobilized PSII on carbonaceous conductors (e.g., carbon nanotube, porous carbon) and semiconductors (e.g., carbon nitride), enhancing charge transfer and stability. This method involves anchoring PSII, extracted from plants (i.e., spinach), onto electrodes with and without polymers for effective integration. Our biohybrid devices, combining PSII-based photoanodes with protease-based cathodes, facilitate water splitting and biophotovoltaic applications with notable efficiency and durability, marking a significant step forward in semi-artificial solar energy conversion systems.

[1] J. Z. Zhang et al., *Nature Review Chemistry*, 4., 6-21 (2020).

[2] W. Tian et al., *Advanced Energy Materials*, 2100911 (2021).

P2: Bilayer nanographene with a benzene defect shows evidence for halide permeation

M. A. Niyas

Uni Wuerzburg, Germany

Understanding permeation of halides through a single benzene defect in graphene is of high importance in the development of halide battery materials, the design of artificial anion receptors or the development of filtration membranes. However, a precise experimental observation of halide permeation so far remained elusive. Here we synthesized a holey nanographene with an atomically precise single benzene pore with a diameter of 1.4 Å. Utilizing supramolecular principles of self-aggregation, we created a kinetically and thermodynamically stable bilayer of the holey nanographene. As the cavity in the holey bilayer nanographene could be accessed only via two angstrom-sized windows, any halide that gets trapped inside the cavity has to permeate through the angstrom-sized single benzene defect. We show the formation of bilayer nanographene and its chloride bound noncovalent complexes using ¹H NMR, MALDI and X-ray crystallography techniques. Our experiments reveal the permeability of fluoride, chloride, and bromide through a single benzene hole, while iodide is impermeable.

P3: CeTa(O,N)₃ and CeNb(O,N)₃ perovskite oxynitrides for photoelectrochemical energy conversion

Gabriel Grötzner^{1,2}, Laura I. Wagner^{1,2}, Lukas Wolz^{1,2}, Verena Streibel^{1,2}, Ian D. Sharp^{1,2}

¹Walter Schottky Institute, TU Munich; ²TUM School of Natural Sciences

Photoelectrochemical (PEC) water splitting presents a promising avenue for the efficient storage of solar energy in chemical bonds. Perovskite oxynitrides, emerging as a promising class of materials for PEC water splitting, hold potential to overcome certain limitations associated with more extensively studied metal oxides. However, the optoelectronic properties of many perovskite oxynitrides are not well understood and investigated. Here we introduce a novel method for synthesizing thin films of the perovskite oxynitrides CeTa(O,N)₃ and CeNb(O,N)₃ through spin coating of liquid phase precursors followed by a two-step annealing procedure in ambient air and ammonia. The investigation explores the structural, compositional

and optoelectronic properties of the thin films and furthermore compares the results between CeTa(O,N)₃ and CeNb(O,N)₃. The experimental findings unveil bandgaps in the visible range and n-type conductivity for both materials. As these results suggest use cases for both materials in PEC water splitting, their viability as photoanodes is also evaluated.

P4: COVALENT ORGANIC FRAMEWORK EMBEDDED WITH SINGLE CU SITES FOR PHOTOCATALYTIC REACTION

Shuo Sun, Jenny Schneider

Ludwig-Maximilians-Universität München, Germany

The development of CO₂ photoreduction catalysts based on covalent organic frameworks (COFs) is an emerging strategy to overcome global energy and sustainability challenges. As porous materials, COFs can serve as light-absorbing carriers in photocatalysis and also provide proper anchoring sites for metal catalysts. By incorporating 2,2'-bipyridine into the COF structure, Cu single atoms can coordinate with the COF materials, which lowers the band gap of the cocatalyst, enhances light harvesting, and promotes charge carrier transport^[1]. This study examines the changes in the photocatalytic properties of photocatalysts with different copper loadings and aims to reveal the formation mechanism of cocatalysts, ultimately improving their performance in photocatalysis.

[1] Zhang, Y., et al., *Small*, 19(22), 2300035 (2023).

P5: EFFECT OF CHAIN LENGTH ON THE PHOTOCATALYTIC HYDROGEN EVOLUTION OF POLYMER-TITANIA HYBRID MATERIALS

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Two hydrophilic conjugated low-band gap copolymers of poly(diketopyrrolopyrrole) and fluorene or carbazole, PDPP[T]₂{TEG}-Flu and PDPP[T]₂{TEG}-Car, were synthesized and characterized. The polymer chain length can be varied by controlling of the monomer ratio. Hybrid materials were formed with titaniumdioxide (TiO₂, anatase) at a ratio of 1:8 (Polymer:TiO₂). On this poster we show, that the activity towards photocatalytic hydrogen evolution increases with the molecular weight of the used polymers. The hybrid materials exhibit a tenfold increase in hydrogen evolution compared to pristine anatase when ethanol is used as a sacrificial agent. Addition of 0.2 wt% Pt show a surface deactivation effect. Furthermore we show, that higher molecular weight of the polymers is beneficial for the hydrogen evolution.

P6: Enhancing Charge Carrier Transport in Metal (Oxy-)Nitrides for Efficient Solar Fuel Generation

Oliver Brune, Laura I. Wagner, Gabriel Grötzner, Ian D. Sharp, Verena Streibel

Walter Schottky Institut, Technische Universität München, Germany

Solar water splitting offers the potential to produce carbon-neutral solar fuels by directly converting sunlight into chemical energy. There exists, however, a scarcity of suitable photoanode materials meeting critical stability and efficiency requirements: long-term chemical stability, high photocarrier extraction efficiency, and appropriate bandgap. An emerging family of photoanode candidates are nitrides and oxynitrides with tunable properties based on cation and anion composition. Promising candidate materials are Ta₃N₅ and LaTiO₂N, exhibiting bandgaps of 2.1 eV but suffering from poor charge carrier transport. To optimize the established

Ta₃N₅, we employ reactive co-sputtering to introduce Zr into Ta₃N₅ thin films and examine how the ternary nitride character of Zr-Ta-N(O) enables improved hole extraction. Various complementary characterization methods reveal that synthesis parameters and Zr content significantly influence the compound's crystal structure, defect concentrations, and (opto-)electronic properties. For the perovskite-type oxynitride LaTiO₂N, the high recombination rate of photoexcited carriers remains a significant challenge. To address this point, we aim to achieve low-defect concentrations within LaTiO₂N thin films using reactive sputter deposition and tailored annealing protocols.

P7: EXPLORING PHOTOINDUCED PHASE SEGREGATION IN MAPBI_{1.5}BR_{1.5} POWDERS

Markus Rainer Griesbach, Fatemeh Haddadi Barzoki, Tobias Siegert, Helen Grüninger, Anna Köhler

University of Bayreuth, Germany

Mixed halide perovskites (MHPs) are prime candidates for multi-junction solar cells due to the tunability of their band gap energy by adjusting the halide composition and many other beneficial optical properties [1]. However, MHPs undergo pronounced halide segregation under illumination, which results in the formation of compositionally heterogeneous phases and ultimately leads deterioration of device performance [2]. Due to the many different factors at play, this process is still not fully understood. In this work, we synthesized a suite of MAPbI_{1.5}Br_{1.5} powders following different synthesis strategies and characterized their properties, which revealed variations in crystallite size and defect density in otherwise very comparable samples. We investigated the phase segregation behavior under illumination by performing in-situ XRD measurements, where we found distinct differences in rate and extent of segregation.

[1] J. Xu *et al.*, Science, 367, 1097-1104 (2020).

[2] E. T. Hoke *et al.*, Chem. Sci., 6, 613-617 (2015).

P8: Facet-dependent photovoltaic efficiency and stability variations in mixed Sn-Pb perovskite solar cells

Xiaoqing Ci, Xiongzhuo Jiang, Guangjiu Pan, Jinsheng Zhang, Zerui Li, Kun Sun, Peter Müller-Buschbaum

Technische Universität München, Germany

Since the first breakthrough of perovskite solar cells by using a solid-state structure, the solar cell's power conversion efficiency has increased from 9.7% to >26%. These exciting improvements are mainly attributed to achieving a pinhole-free thin film at the beginning and an increased understanding of microstructures on perovskite thin films. Nevertheless, the deep understanding of perovskite thin films, especially the crystal facets of the thin film, still lags behind that of single-crystal samples or other inorganic thin films. In this work, we prepare the mixed tin-lead perovskite film with different orientations according to the facet engineering. We research the role of the different perovskite crystal facets in stability and optoelectronic properties.

P9: FUNCTIONAL HIERARCHICAL SUPERSTRUCTURES FOR (PHOTO-) CATALYSIS

Dennis Schröder

University of Bayreuth, Germany

To advance the frontiers of nanotechnology, it is essential to devise more sophisticated and accurate processing techniques to enhance the functionality of devices. In this study, we present a versatile process for the creation of functional hierarchical superstructures using physical vapor deposition. The functionality of the superstructures can be specifically controlled through the rational design of the components utilized. It has been demonstrated that superstructures can be produced that are suitable for immobilizing metal nanoparticles and can be used as heterogeneous catalysts by using functionalized benzene trisamides.[1] Secondly, we demonstrate that superstructures can be produced using tricycloquinazoline, which can then be employed as photocatalysts, for example, to remove organic pollutants from wastewater.[2] The versatility of the process allows for the creation of new superstructures and their use in applications, like filtration or reinforcement materials.

[1] D. Schröder *et al*, *Adv. Mater. Interfaces.*, 2024, 2400259. <https://doi.org/10.1002/admi.202400259>

[2] D. Schröder *et al*, *Small Sci.*, 2024, 4, 2300160. <https://doi.org/10.1002/smssc.202300160>

P10: GIWAXS STUDIES OF 2D RUDDLESDEN–POPPER PEROVSKITES FOR PHOTOMEMRISTORS APPLICATIONS

Christopher Greve¹, Po-Ting Lai², Cheng-Yueh Chen², Bo-Yuan Chuang³, Kai-Hua Kuo³, Tsung-Kai Su², Guang-Hsun Tan², Chia-Feng Li⁴, Sheng-Wen Huang⁴, Kai-Yuan Hsiao², Eva M. Herzig¹, Ming-Yen Lu², Yu-Ching Huang⁴, Ken-Tsung Wong³, Hao-Wu Lin²

¹Universität Bayreuth, Germany; ²National Tsing Hua University, Taiwan; ³National Taiwan University, Taiwan; ⁴Ming Chi University of Technology, Taiwan

We investigate 2D Ruddlesden–Popper (RP) perovskites incorporating a highly polar donor–acceptor-type organic cation, EATPCN⁺, implemented in ultrasensitive photomemristors as charge-trapping layers. (EATPCN)₂PbI₄ devices exhibit high linearity and almost zero-decay retention, outperforming traditional 2D RP (i.e. OA⁺ and PEA⁺ based) and 3D perovskite devices. The superior performance is attributed to optimized crystal arrangement, deduced from GIWAXS, and an optimized band alignment via the organic cation. The photomemristor devices show an impressive memory window, on/off ratio, and exceptional retention, with extremely low energy consumption and high photosensitivity. Additionally, these photomemristors accurately reconstruct images and achieve high accuracy in image recognition tasks, marking a significant advancement in perovskite-based photomemristors.

P11: Hierarchical electrostatic nanotemplating and self-assembly of electron-transferring hybrid nanostructures for Photocatalysis.

Jyoti Devi, Maximilian Wagner, Franziska Gröhn

Friedrich Alexander university Erlangen-Nuremberg, Germany

Inspired by the photosynthesis of plants in Mother Nature, self-assembled photocatalysts are highly desirable, in particular in aqueous environments. Spontaneous electrostatic self-assembly in water can lead to the functional interconnection of different molecular components, where supramolecular nano-objects with various shapes can form. Furthermore, polyelectrolytes or their assemblies can yield organic-inorganic hybrid particles by electrostatic nanotemplating. Both approaches – electrostatic self-assembly and electrostatic nanotemplating – can be combined to create more complex, hierarchical, functional and adjustable multi-component nano-objects (Fig.1).

In this contribution, photocatalytically active multicomponent nano-objects consisting of macroions and oppositely charged species will be presented. By self-assembly, the photocatalytic activity of the active species can be enhanced and photocatalytic selectivity can be achieved. For example, a polyelectrolyte can connect semiconductor nanoparticles with a porphyrin as a light harvester, such that a larger range of the (solar) spectrum is exploited. Key for targeted applications is to understand structure directing effects. This again involves a detailed characterization on the nanoscale by light and small-angle scattering (SLS, DLS, SANS, SAXS), atomic force microscopy (AFM), transmission electron microscopy (TEM) and on a molecular level by spectroscopy, in conjunction with analyzing the self-assembly thermodynamics and interplay of interaction forces by isothermal titration calorimetry (ITC). Structure-function relationships will be discussed.

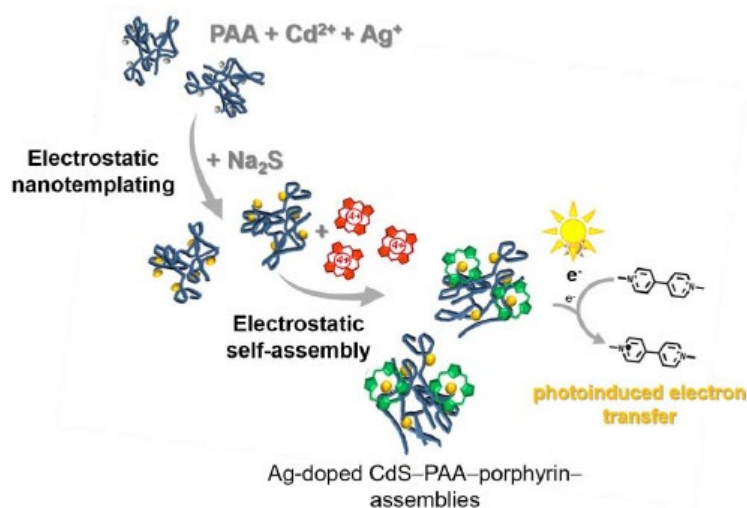


Fig. 1. Hierarchical electrostatic templating – electrostatic self-assembly approach yielding catalytically active nano-objects: Silver-doped cadmium sulfide-poly(acrylic acid)-porphyrin assemblies.

Krieger, A.; Zika, A.; Gröhn, F. *Frontiers in Chemistry* **2022**, *9*, 779360 (Review Article). / Düring, J.; Hölzer, A.; Kolb, U.; Branscheid, R.; Gröhn, F. *Angew. Chem. Int. Ed.* **2013**, *52*, 8742. / Mariani, G.; Moldenhauer, D.; Schweins, R.; Gröhn, F. *J. Am. Chem. Soc.* **2016**, *138*, 1280. / Zika, A.; Agarwal, M.; Schweins, R.; Gröhn, F. *Chemistry - A Eur. J.* **2023**, *29*, e202203373. / Zika, A.; Agarwal, M.; Zika, W.; Guldj, D.; Schweins, R.; Gröhn, F. *Nanoscale* **2024**, *16*, 923. / Krieger, A.; Wagner, M.; Haschke, S.; Kröckel, C.; Bachmann, J.; Hauke, F.; Hirsch, A.; Gröhn, F. *Nanoscale* **2020**, *12*, 22952. / Wagner, M.; Strassert, C. A.; Gröhn, F. *Nanoscale* **2022**, *14*, 13040. / Wagner, M.; Gröhn, F. *Catalysts* **2022**, *12*, 907. / Bernhardt, S.; Yokosawa, T.; Spiecker, E.; Gröhn, F. *Langmuir* **2023**, *39*, 10312. / Bernhardt, S.; Wagner, M.; Gröhn, F. *ACS Appl. Nano Mater.* **2022**, *5*, 12380.

P12: Highly Crystalline Oriented (NOP)₄AuB₃I₈ Gold-based Ruddlesden Popper 2D Double Perovskite thin films as Photodetectors

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We present three novel (NOP)₄AuB^{III}I₈ gold-based Ruddlesden Popper 2D perovskites incorporating naphthalene-O-propylammonium cation as conductive organic cation. All three materials form highly crystalline thin films, oriented along the [001] direction on both FTO and glass substrates. They show strong optical absorption in the visible spectrum along with

feasible charge carrier mobilities and lifetimes. Their potential application as photodetector was demonstrated through photoconductivity measurements, which revealed 12 times increased electrical conductivity under 1 sun illumination.

P13: Improved Control of Perovskite Thin Film Fabrication via Reactive Spin coating based on Real-Time In-Situ Feedback from Optical Spectroscopy

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Efficient solar cells require a high-quality halide perovskite (HP) film, which is typically achieved through a solution-based solvent engineering spin coating approach. Here, HP crystallization is induced by applying an antisolvent (AS) to the precursor solution film on the spinning substrate after a specific spinning time. The process involves various controllable and uncontrollable parameters that need to be considered. As a result, fabrication recipes (such as spin speed or timing of AS dispensing) are usually developed empirically and vary between labs. Additionally, factors like changes in the atmosphere that are hard to control can introduce substantial variations between and even within batches of devices. In this work, we developed a closed-loop feedback system based on our multimodal optical In-Situ spin coater system in combination with real-time analysis of the optical spectra during spin coating. We monitor the solvent layer thickness as the parameter of interest during the spin coating. When the target level is reached, the HP crystallization is induced by dispensing the AS via a syringe pump. This method compensates for the effects of uncontrolled parameters, like variation in solvent evaporation rate due to atmospheric changes, thus, leading to reproducible film quality.

P14: INFLUENCE OF SECOND SPHERE MODIFICATIONS ON THE PERFORMANCE OF PORPHYRIN PHOTOCATALYSTS FOR CO₂ REDUCTION

Peter Stahl, Christian Wilhelm, Ivana Ivanović-Burmazović
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Porphyrins with a modifications in the second coordination sphere have shown great promise for photocatalytic CO₂ reduction [1]. To further investigate the influence of these groups, a library of charged porphyrins and of crown ether functionalized porphyrins was synthesized and their performance under standard photochemical CO₂ reduction conditions was evaluated.

[1] Robert et al, *Nature*, 548, 74 (2017).

P15: Interferometric Scattering in Battery Materials

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Understanding electrochemical processes at the nanoscale is crucial for developing advanced nanomaterials for energy technologies. While current observations predominantly focus on bulk properties, there is limited understanding at the single-nanoparticle level. Hence, the visualization of the underlying mechanisms, such as ion transport and charge transfer, is a promising target for gaining insights into fundamental energetic and kinetic factors driving these processes. Interferometric scattering (iSCAT) microscopy offers a solution by enabling label-free optical sensing of nanoscale processes with high speed and precision [1,2]. This technique holds significant potential for investigating battery materials, particularly 2D materials, such as transition metal carbides, carbonitrides and nitrides (MXenes) [3]. By coupling iSCAT with an electrochemical reactor, we can visualize nano-processes such as ion diffusion in MXene nanostructures. This has revealed critical factors influencing the power density and contributing

to the lifetime of these promising battery materials.

[1] J. Ortega Arroyo, P. Kukura et al, *Nature Protocols*. 11, 617-633 (2016).

[2] C. Gruber, E. Cortés et al, *Nature*. 630, 872–877 (2024).

[3] B. Anasori, Y. Gogotsi et al, *Nature Reviews Materials*. 2, 16098 (2017).

P16: INVESTIGATING GIANT ELECTROSTRICTION IN HALIDE PEROVSKITES WITH DOUBLE MODULATION INTERFEROMETRY

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The discovery of materials with giant electrostriction has sparked significant interest due to its magnitude, which is much greater than expected based on the materials mechanical and dielectric properties. This effect occurs at low frequencies and is often linked to defects in the material.¹ Metal halide perovskites, known for their high power conversion efficiency in solar cells, have also shown a giant electrostrictive effect.² In this study, we examine the electrostriction of various perovskite samples with different morphologies, including MAPbI₃ and MAPbBr₃ single crystals, thin films, aerosol deposited thick films, and powder based pellets. To do this, we developed a novel interferometer using the iLens method and enhanced it with double modulation.³

[1] Y. Jiacheng et al, *Journal of Applied Physics* 131.17 (2022).

[2] B. Chen et al, *Nature materials* 17.11, 1020-1026 (2018).

[3] M. Pooja et al, *Applied Physics Letters* 115.11 (2019).

P17: Investigation of Binding Motifs in Bioinspired Semisynthetic Zinc Chlorin Aggregates

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Semisynthetic zinc chlorins are significant due to their potential to mimic the efficient light-harvesting properties of natural chlorosomes. The bioinspired aggregates based on zinc chlorin (ZnChl) form well-defined single-walled tubular structures, as revealed by polarized resolved spectroscopy [1], AFM and TEM research [2]. We present an investigation of the fundamental binding structure of zinc chlorin molecules, examining the effects of the central atom and the altered substituents in comparison to the naturally occurring bacteriochlorophyll c molecules found in chlorosomes.

[1] A. Löhner et al, *J. Phys. Chem. Lett.*, 10, 2715 (2019)

[2] S. Sengupta et al, *Angew. Chem., Int. Ed.* 51, 6378– 6382 (2012)

P18: IRON-DOPED PEROVSKITE CRYSTAL GROWTH FOR ADVANCED OPTOELECTRONIC AND SPINTRONIC APPLICATIONS

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While semiconducting perovskite materials have been extensively studied for photovoltaic and light-emitting applications, little is known about the magnetism of this class of materials. Doping perovskite materials with transition metal ions can enhance their potential and open perspectives for spintronic applications [1]. This study focuses on the growth of lead-based (MAPbCl₃, MAPbBr₃, MAPbI₃) and lead-free (Cs₂AgBiBr₆) perovskite single crystals, doped with Fe²⁺ and Fe³⁺ at various doping concentrations. The Fe-doped single crystals were successfully

grown by inverse temperature crystallization and controlled cooling crystallization techniques, allowing the precise control over crystal formation, which is crucial for optimizing material properties. Various characterization methods were applied to investigate the impact of Fe²⁺ and Fe³⁺ ions on crystal structure, as well as optical and magnetic properties of perovskite single crystals, and the first results are presented here.

[1] W. Ning et al., *Science Advances*, vol. 6, no. 45 (2020).

P19: Lateral π -extended molecular nanographene

Giovanni M. Beneventi¹, Kilian Schöll¹, Fabrizia Negri², Alejandro Cadranell¹, Norbert Jux¹, Dirk M. Guldi¹

¹Friedrich-Alexander-Universität, Germany; ²Department of Chemistry "Giacomo Ciamician"

Molecular nanographenes represent a promising candidate for optoelectronics and energy applications, in view of their intriguing and tunable properties. We report [1] on the rich photophysics and self-assembly behaviour of two nitrogen-doped nanographenes: azananographene sP, which features a hexa-peri-hexabenzocoronene (HBC) core, and diazananographene NG, which can be regarded as a laterally pi-extended HBC. Our work was rounded off by coordinating ruthenium porphyrins (RuP) to the nitrogen centers of sP and NG, leading to sP-RuP and RuP-NG-RuP. The lateral π -extension of the aromatic core when going from sP to NG, resulted in an intriguing modulation of the photophysical properties, allowing anti-Kasha emission and "ping-pong" energy transfer cascade, along with the rise of self-assembly behaviour into 2D supramolecular polymers.

[1] G.M. Beneventi et. al. *Adv. En. Mat.* 14, 2401529 (2024).

P20: LIGHT-DRIVEN Mn-PORPHYRIN NANOASSEMBLY FOR CATALYSIS

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Self-assembled nanostructures offer significant potential in fields like drug delivery, sensors, catalysis, and solar energy conversion [1,2]. Their formation is driven by secondary interactions, e.g. electrostatic forces and hydrogen bonding. Moreover, polymer-based supramolecular structures, which rely on non-covalent interactions rather than covalent bonds, are a growing area at the intersection of polymer science and supramolecular chemistry [3,4]. Here, a cationic polyelectrolyte-templated Mn(III) porphyrin (Mn(III)P) nanoassembly is proposed as a catalyst via photoinduced electron transfer (PET). The protonation degree and chain flexibility of the polyelectrolyte are key to controlling the electron transfer and tuning the redox activity of Mn(III), allowing for the creation of stable Mn(III)P nanoparticles for catalytic use.

[1] S. Chang et al., *Crystals*, 12(2), 274 (2022).

[2] L. Varma et al., *Current Drug Delivery*, 17(4), 279-291 (2020).

[3] M. Wagner et al., *Catalysts*, 12, 907 (2022).

[4] J. F. Stival et al. *Applied Catalysis A: General*, 662, 119271 (2023).

P21: Mechanistic Insights of Tunable Iridium(III) Complexes as Sensitizers for Organic Photocatalysis via Triplet-triplet Energy Transfer

Lukas Alexander Mai

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A valuable mechanism in organic photocatalysis has been triplet-triplet energy transfer (TTE_nT) catalysis.^[1] For an effective energy transfer towards different molecules, tunable

photosensitizers are eminent. Cyclometalated Ir(III) complexes have shown to be not only tunable, but also efficient triplet-triplet energy transferring photosensitizers.^[2] Combined with a reaction- and mechanism-based screening approach, we achieved various novel synthesis routes. Though, the mechanism of the can be very complicated and is under continuous investigation. We provide new insights, elucidate emerging equilibria and eliminate unwanted reaction pathways.

[1] Felix Strieth-Kalthoff et al, *Chem. Soc. Rev.* **2018**, *47*, 7190-7202.

[2] T. Paulisch, Lukas Mai et al, *Angew. Chemie, Int. Ed.* **2022**, *61*, e202112695

P22: MULTIPLY-FUSED PORPHYRIN-NANOGRAPHENE CONJUGATES

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The application of porphyrins as a main element for the design of extended carbon-based frameworks has gained increasing popularity in recent years. The fusion of aromatic hydrocarbons of various sizes to the β - and *meso*-positions of porphyrins emerged hereby as a particularly convenient strategy for an effective expansion of the aromatic network.^[1] The here-presented extension of the π -system leads to substantial alterations in optical and electrochemical features. These changes involve a bathochromic shift in the absorption spectrum, increased absorption in the NIR range, and a profound decrease of the HOMO-LUMO gap.^[2]

[1] A. Borissov et al., *Chem. Rev.* **2022**; *122*: 565–788.

[2] C. Oleszak, P. R. Schol, C. L. Ritterhoff, M. Krug, M. M. Martin, Y. Bo, B. Meyer, T. Clark, D. M. Guldi, N. Jux, *Angew. Chem. Int. Ed.* **2024**, accepted; DOI: 10.1002/anie.202409363

P23: Nanostructure in energy materials

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(no abstract submitted)

P24: PHOTOPHYSICAL PROPERTIES OF CYLINDRICAL MOLECULAR AGGREGATES FOR LIGHT-HARVESTING APPLICATIONS

Lisa Maria Günther¹, Stefan Goppelt¹, Tenzin Kunsel², Thomas L. C. Jansen², Jasper Knoester^{2,3}, Jürgen Köhler¹

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Features like fast and efficient energy transfer, non-linear optical behavior and tunability of spectral properties make low-dimensional organic supramolecular structures promising candidates for the development of new optoelectronic devices with tailored properties. The elementary electronically excited states of such systems are delocalized excitons. Since the photophysical properties of such systems are intrinsically linked to their geometric structures, assemblies of cylindrical shape feature favorable characteristics for light-harvesting and energy transport. We provide a systematic description of the relationships between various parameters, such as radius, length, geometrical arrangement of the molecular building blocks, structural and energetic disorder, and the optical observables.

P25: Precision excited state calculations in small metal clusters: prototypes for future photocatalytic applications

Nikita Kavka, Simon Herb, Roland Mitric

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When metals are scaled down to nanosized clusters, they exhibit unique properties that diverge significantly from those observed in bulk materials. At this scale, quantum effects become prominent, leading to distinct electronic structures and enhanced reactivity. These characteristics make small metal clusters valuable for photocatalysis, such as water splitting and CO₂ reduction. Understanding their electronic structures and excited states is key to advancing these applications. Our research employs advanced *ab initio* multi-reference computational methods to study the excited states of clusters like Au₃⁺, Ce₂, and Cu₂. By combining our theoretical studies with various experimental techniques, we provide fundamental data that could enhance the development of improved photocatalytic materials.

P26: Production of Thin Films with Inverse Opal Structure via Soluble Alloy Based Precursors

Aimilios Christidis, Christian Fajman, Katja Rodewald, Christian Weindl, Guangjiu Pan, Peter Müller-Buschbaum, Thomas Fässler

TUM School of Natural Sciences, Germany

The recent development forming OER catalysts from polar intermetallic alloys or Ni₂Si hybrid materials from *Zintl* phases, inspired our interest in transferring such ideas to well-defined nanostructured materials.[1,2] Several years ago, we developed a synthetic route by infiltrating polymethyl methacrylate (PMMA) opals with a diameter between 250 and 300 nm and reactive soluble intermetallic precursors comprising soluble Ge₉₄- and Sn₉₄- Clusters.[3,4] Here we report on the transfer of the synthetic protocol applying using mixed atom clusters [Tm@Ge₉]x- and [Tm@Sn₉]x- and the formation of inverse opal structures. For example, using the endohedrally filled *Zintl* clusters such as [NiSn₉]⁴⁻ we aim to retain catalytically active Ni (0) species in the Ni/Sn inverse opal structure.

[1] Menezes *et al.*, *Adv. Mater.* 33, 2008823 (2021); [2] Polterhault *et al.*, *Nanoscale* 648, 15209-15213 (2020); [3] T. F. Fässler *et al.*, *Angew. Chem. Int. Ed.* 55, 2441-2445 (2016); [4] T.Fässler *et al.*, *Z. Anorg. Allg. Chem.* 648, e202100362 (2022).

P27: Vibrational Anharmonicity and Optoelectronic Properties of 2D Perovskites

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2D halide perovskites are a highly promising class of materials for solar energy conversion, for which connections of electronic and vibrational properties have not been fully studied yet. For 3D perovskites, it has been observed that vibrational anharmonicity significantly affects the band gap and electronic structure [1]. In this work, we investigate the lattice dynamics of (BA)₂PbI₃ from molecular dynamics (MD) calculations which include anharmonic vibrations. We combine this with a real-space model to predict the electronic structure and bonding contributions depending on structural disorder. This allows us to evaluate the dynamic electronic properties of 2D perovskites in comparison to 3D perovskites. Specifically, we investigate connections between vibrational anharmonicity, bonding, and electronic structure at finite temperature.

[1] Seidl, S. A. et al, *Phys. Rev. Mater.* 7, L092401 (2023)

P28: Selective Synthesis of Graphene Nanoribbons and the Corresponding Porphyrin Conjugates

Filip Bozinovic, Norbert Jux

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The physical properties of graphene and smaller nanographene are influenced by their size, shape and edge structure. However, since most synthetic approaches towards nanographene lack of control on the above-mentioned structural features, we herein introduce a new strategy towards well defined graphene nanoribbons.[1] A coupling to porphyrins leads to a new compound class with remarkable photophysical properties, such as energy transfer between both chromophores.[2]

[1] K. Müllen et al, *Angew. Chem. Int. Ed.*, 51, 7640-7654 (2012).

[2] N. Jux et al, *Chem. Eur. J.*, 24., 15818-15824 (2018).

P29: Simulating anisotropic photo-physical properties of plexcitons

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University of Würzburg, Germany

Plexcitons are quasi particles, which arise by the strong-coupling of surface plasmon polaritons and electronically excited states of molecules. Due to their versatile properties, plexcitons are potential candidates for new photonic applications. In this study, we investigate thin films of self-assembled oriented J-type liquid crystalline perylene bismide (PBI) molecules, arranged in a three-stranded helical structure [1], on a silver surface. Measured plexciton dispersions of absorption and emission show a distinct angle anisotropy. We employ TD-DFT calculations to investigate the angular-dependence of the plexcitonic dispersion. Furthermore, we propose a simple model to simulate photoluminescence spectra of plexcitonic samples. Understanding the connection between the supramolecular structure and the anisotropic optical properties is fundamental for future applications of metal-organic hybrid structures.

[1] S. Herbst et al, *Nat. Commun.* 9(1), 2646-2654 (2018).

P30: SPUTTER-DEPOSITED TiO_x THIN FILM AS A BURIED INTERFACE MODIFICATION LAYER FOR EFFICIENT AND STABLE PEROVSKITE SOLAR CELLS

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It is crucial to suppress the non-radiation recombination in the hole-blocking layer (HBL) and at the interface between the HBL and active layer for performance improvement. We deposited a TiO_x thin layer atop the SnO₂ layer via sputter deposition at room temperature as an interface modification layer. The structure evolution of TiO_x during sputter deposition is investigated via in situ grazing-incidence small-angle X-ray scattering (GISAXS). The HBL, combined with the TiO_x interface modification layer, shows a suitable transmittance, smoother surface roughness, and fewer surface defects, thus resulting in lower trap-assisted recombination at the interface between the HBL and the active layer. With the sputter-deposited TiO_x buried interface modification layer, the perovskite solar cells exhibit higher power conversion efficiencies and stability than the unmodified SnO₂ monolayer devices.

P31: SUPPRESSED DEGRADATION PROCESS OF PBDB-TF-T1:BTP-4F-12 SOLAR CELLS WITH SOLID ADDITIVE EH-P

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¹Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany; ²Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, WACKER Chair of Macromolecular Chemistry, Lichtenbergstrasse 4, 85748 Garching, Germany;

³Deutsches Elektronen-Synchrotron, Notkestrasse 85, 22607 Hamburg, Germany

Solid additives have garnered significant attention due to their numerous advantages over liquid additives. In this study, we explore the potential of the polymer EH-P as a solid additive in green-solvent based PBDB-TF-T1:BTP-4F-12 solar cells. Even tiny amounts of EH-P doping significantly improve device performance. For the reference solar cell without any additive, we found that cell device degradation is not caused by chemical reoxidation, but by changes in crystallinity and microstructure evolution during aging in air under illumination. Operando GIWAXS and GISAXS are used to investigate this structure evolution. We discovered a three-stage degradation process for the reference cell, and EH-P doping effectively suppresses the evolution of crystallinity and domain sizes, thereby enhancing device stability under illumination in air. This demonstrates the promising potential of EH-P doping in the field of solar cell technology.

P32: Surface Enhanced IR Absorption Spectroscopy to Study the CO₂ Reduction Reaction (CO₂RR) on Gold Nanostructures

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The urgent need to mitigate climate change has driven significant research into carbon dioxide reduction reaction (CO₂RR) technologies. Surface-enhanced infrared absorption spectroscopy (SEIRAS) is a robust method for evaluating electrocatalysts due to its ability to probe surfaces in a non-destructive, chemically sensitive, and in-situ manner [1]. In this research, we study thin Gold films as a catalyst, and investigate surface dynamics due to the presence of nanostructures using SEIRAS. Previous work done in our group has shown a drastic increase in SEIRAS signals through the use of a Platinum nano-slot metasurface [1]. Here we use Gold electrodes, which have the benefit of being highly selective in the CO₂RR to CO [2]. The goal of our research is to gain a deeper insight to CO₂RR mechanism on Gold surfaces. Therefore we developed a procedure to stabilize thin Gold films, design nanostructures for SEIRAS enhancement and obtained clean conditions.

[1] L. M. Berger, M. Duportal, L. de S. Menezes, *Adv. Funct. Mater.* 2023, 33, 2300411.

<https://doi.org/10.1002/adfm.202300411>

[2] S. Mezzavilla, S. Horch, I. E. L. Stephens, B. Seger, I. Chorkendorff, *Angew. Chem. Int. Ed.* 2019, 58, 3774.

P33: Synthesis and Characterization of Expanded Azaborahelicenes

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Julius-Maximilians-Universität Würzburg

Helicenes are a group of non-planar polycyclic aromatic hydrocarbons (PAHs) exhibiting appealing electronic and optoelectronic properties and therefore showing potential for applications in organic electronics. These compounds have been investigated as

semiconductors in organic field-effect transistors (OFETs) and as spin filters.[1,2] More recently, they have been intensively studied as chiral emitters in state-of-the-art circularly polarized organic light emitting diodes (CP-OLEDs) where the use of compound showing circularly polarized light (CPL) emission is proposed as a method to increase the light outcoupling efficiency.[3] Among the factors that can influence helicene properties, the three most important are: 1) the helical and lateral extension of the helical structure,[4] 2) the presence of heterocycles in the molecular skeleton,[5] and 3) the ring connection pattern (angularly or linearly fused rings).[6] As previously proposed,[7] we aim to combine these three components to enhance the optical properties of the resulting molecules. The poster will present our ongoing research on expanded azaborahelicenes, including their synthesis by previously described modular approach.[7]

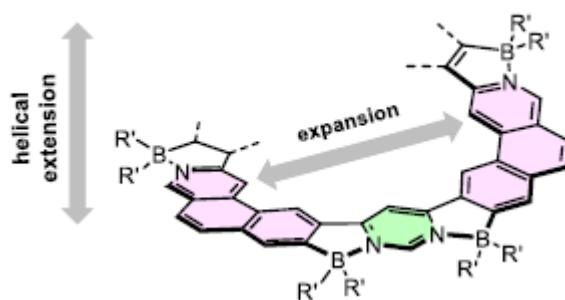


Figure 1. General molecular structure of target extended azaborahelicenes.

- [1] L. Zhang, I. Song, J. Ahn., M. Han, M. Linares, M. Surin, H.-J. Zhang, J. H. Oh, J. Lin, *Nat. Commun.* 12, 142 (2021).
 [2] M. Kettner, V. V. Maslyuk, D. Nürenberg, J. Seibel, R. Gutierrez, G. Cuniberti, K.-H. Ernst, H. Zacharias, *J. Phys. Chem. Lett.* 9(8), 2025-2030 (2018).
 [3] K. Dhbaibi, L. Abella, S. Meunier-Della-Gatta, T. Roisnel, N. Vanthuyne, B. Jamoussi, G. Pieters, B. Racine, E. Quesnel, J. Autschbach, J. Crassous, L. Favereau, *Chem. Sci.* 12, 5522-5533 (2021).
 [4] F. Full, Q. Wöflück, K. Radacki, H. Braunschweig, A. Nowak-Król, *Chem. Eur. J.* 28, e202202280 (2022).
 [5] K. Dhbaibi, L. Favereau, J. Crassous, *Chem. Rev.* 119, 8846-8953 (2019).
 [6] G. R. Kiel, H. M. Bergman, A. E. Samkian, N. J. Schuster, R. C. Handford, A. J. Rothenberger, R. Gomez-Bombarelli, C. Nuckolls, T. D. Tilley, *J. Am. Chem. Soc.* 144 (51), 23421-23427 (2022).
 [7] J. Full, S. P. Panchal, J. Götz, A.-M. Krause, A. Nowak-Król, *Angew. Chem. Int. Ed.* 60, 4350 (2021).

P34: TOWARDS CD-SPECTROSCOPY OF SINGLE CHLOROSOMES

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The light-harvesting aggregates of green-(non)-sulfur bacteria, so called chlorosomes belong to the most efficient light-harvesting systems in nature. Owing to their collection efficiency these serve as templates for novel solar cells [1]. Chlorosomes are phospholipid sacks that are filled with BChl molecules that form molecular aggregates. In these aggregates the molecules are arranged in secondary structural elements that feature predominantly cylindrical motifs. Details such as curvature and length of these elements can be obtained from polarization-resolved spectroscopy and in particular by circular-dichroism spectroscopy [2]. Given the structural heterogeneity within an ensemble of chlorosomes these techniques are most beneficial for single chlorosomes.

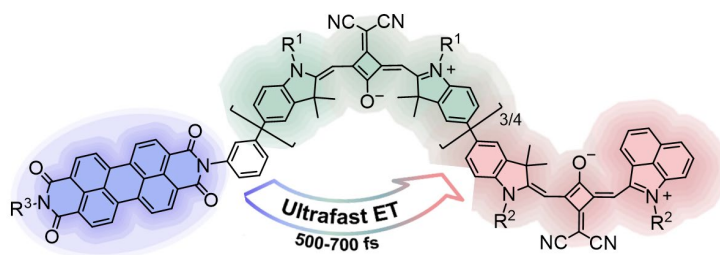
- [1] S. Sengupta et al, *Angew. Chem. Int. Ed.*, 51: 6378-6382 (2012)
 [2] T. Kunsel et al, *J. Chem. Phys.* 155, 124310 (2021)
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P35: Ultrafast Energy Transfer in Squaraine Oligomers

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Building on an established synthetic strategy using protecting groups^[1] we developed a method for the linear synthesis of donor-acceptor substituted squaraine oligomers. These donor-acceptor systems with up to four bridging squaraine units form a random coil or a helix superstructure depending on the solvent.^[1] fs-Transient absorption spectroscopy prove ultrafast energy transfer from the PDI to the acceptor on the order of several hundred femtoseconds. We are aiming to gain further insight into the energy transfer mechanisms between the respective moieties, by changing the oligo-squaraine bridge length, as well as donor and acceptor.



[1] Lambert et al., *Chem. Eur. J.*, **2021**, 27, 8380-8389.
