AGENDA

15th SolTech International Conference in Munich

November 9 – 11, 2026

SOLAR TECHNOLOGIES go HYBRID

hbw ConferenceCenter Haus der Bayerischen Wirtschaft

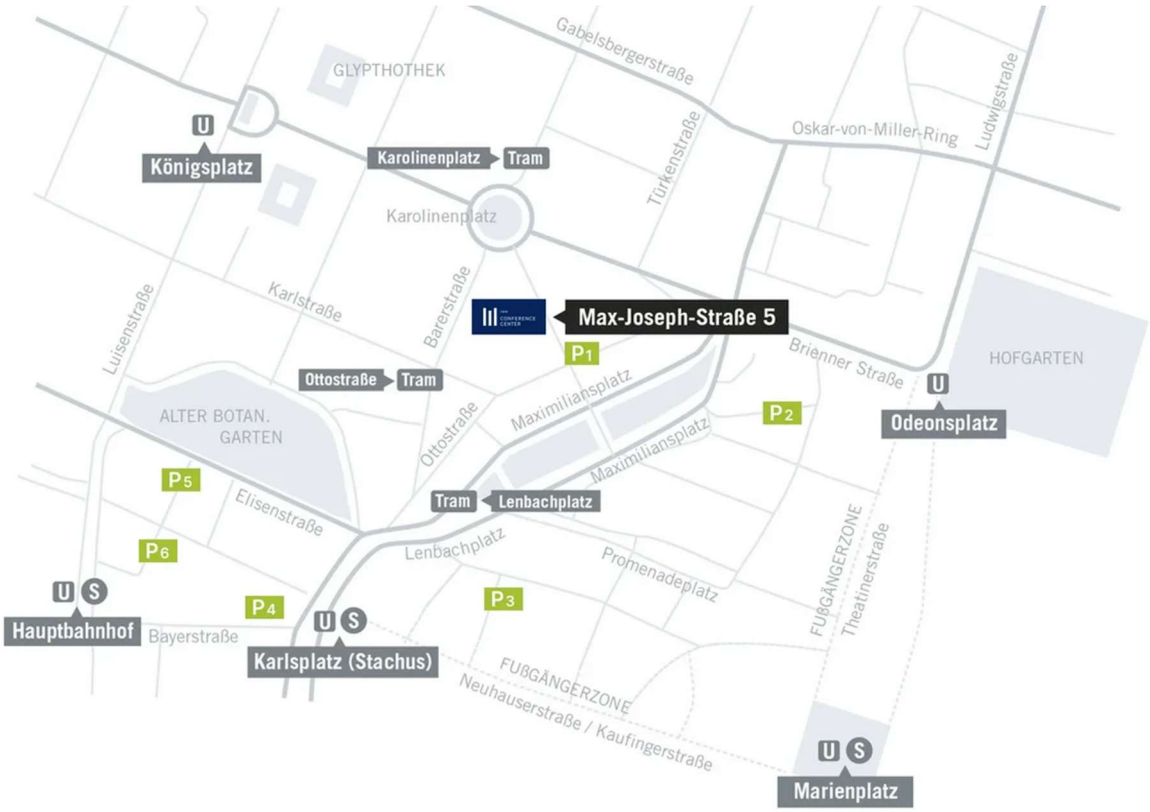
Max-Joseph-Straße 5, 80333 München



Solar Technologies Go Hybrid - KeyLabs

Universität Bayreuth
Julius-Maximilian-Universität Würzburg
Friedrich-Alexander-Universität Erlangen-Nürnberg
Technische Universität München
Ludwig-Maximilian-Universität München

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Acknowledgement

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Bayerisches Staatsministerium für Wissenschaft und Kunst

Monday, November 9, 2026

12:30 – 13:00 Arrival and Registration

Session 1 Chair: Frank Würthner (JMU)

13:15 **Peter Müller-Buschbaum** (TUM)

OPENING REMARKS

13:30 **Invited Speaker: Jochen Feldmann** (LMU, Physik)

SOLTECH HISTORY

13:50 **Johannes Brendel** (UBT)

DESIGNING CONJUGATED POLYELECTROLYTES FOR OPTOELECTRONIC APPLICATIONS

14:10 **Vishnu Eyyanikattil Krishnan** (JMU)

DISENTANGLING NONLINEAR SIGNAL ORDERS IN FLUORESCENCE-DETECTED MULTIDIMENSIONAL SPECTROSCOPY VIA INTENSITY CYCLING

14:30 **Alejandro Cortes Villena** (FAU)

PEROVSKITE NANOCRYSTAL HYBRIDS AS TUNABLE PLATFORMS FOR ENERGY AND CHARGE TRANSFER

14:50 – 15:30 Coffee Break

Session 2 Chair: Jochen Feldmann (LMU)

15:30 **Invited Speaker: Michael Saliba** (Institut für Photovoltaik, Universität Stuttgart)

SHEDDING LIGHT ON WIDE-BANDGAP PEROVSKITES

16:10 **Alexander Urban** (LMU)

ALGORITHMS AND ANTISOLVENTS: THE ART OF BUILDING PERFECT 2D NANOPLATELETS

16:30 **Manjari Jain** (TUM)

PREDICTING THE ELECTRONIC STRUCTURE OF HALIDE PEROVSKITE SURFACES AND NANOSTRUCTURES USING PHYSICS INFORMED HAMILTONIAN LEARNING

16:50 – 18:00 **Poster Session I** (Poster no 1-21)

18.00 – 20.00 Get Together (Beer, Pretzel, Finger food)

Tuesday, November 10, 2026

Session 3 Chair: Johannes Brendel (UBT)

09:00 **Invited Speaker: Alexander Kuehne** (Organic Chemistry, Universität Ulm)

ORGANIC MOLECULES FOR PHOTONIC AND QUANTUM TECHNOLOGIES

09:40 **Agnieszka Nowak-Krol** (JMU)

CHIRAL BN-CONTAINING PAHS: FROM DESIGN AND SYNTHESIS TO FUNCTION

10:00 **Anna Köhler** (UBT)

DISENTANGLING EXCITON DISSOCIATION PATHWAYS IN THE NON-FULLERENE ACCEPTOR Y6

10:20 – 11:00 Coffee Break

Session 4 Chair: Ian Sharp (TUM)

11:00 **Norbert Jux** (FAU)

ARYL-FUSED PORPHYRINS

11:20 **Hagen Übele** (TUM)

HOW COPPER OXIDATION IMPACTS THE INTERFACIAL pH AND THEREBY STEERS PRODUCT SELECTIVITY IN PULSED CO2 REDUCTION ON COPPER ELECTRODES

11:40 **Jan Gerrit Horstmann** (JMU)

GOOD VIBRATIONS: OPTO-STRUCTURAL CONTROL OF FUNCTIONAL MATERIALS

12:00 **Lisa Günther** (UBT)

TIME-RESOLVED FLUORESCENCE SPECTROSCOPY FOR RESEARCH ON SOLAR TECHNOLOGIES: A KEYLAB APPROACH

12:20 – 13:30 Lunch Break

Session 5 Chair: Bettina Lotsch (LMU)

13:30 **Student Highlights** (5 talks, five min. each, 5 min discussion): Markus Griesbach (UBT),

Giovanni Mariano Beneventi (FAU), Zehua Xu (LMU), Martin Schwade (TUM), Mathilde Seinfeld (JMU)

14:10 **Invited Speaker: Doug Fabini** (PSI)

A SIMPLE PHYSICAL MODEL FOR CHEMICAL CONTROL OF DISORDER AND DYNAMICS IN HYBRID PEROVSKITE ENERGY MATERIALS

14:50 **Esma Ugur** (LMU)

PEROVSKITE TANDEM SOLAR CELLS: FROM EFFICIENCY TO STABILITY

15:10 **Zhaonan Jin** (TUM)

ALKALI AND SCN ⁻ADDITIVE ENGINEERING FOR ENHANCED LATTICE STABILITY IN WIDE-BANDGAP INVERTED PEROVSKITE SOLAR CELLS

15:30 – 16:00 Coffee Break

Session 6 Chair: Thomas Fässler (TUM)

16:00 **Invited Speaker: Uli Lemmer** (Lichttechnisches Institut, KIT)

PRINTED ENERGY CONVERSION DEVICES

16:40 **Lirong Dong** (FAU)

UPSCALLING OF FLEXIBLE PEROVSKITE SOLAR MODULES

17:00 **Jenny Schneider** (LMU)

SINGLE-METAL-SITES IN COFS FOR PHOTO- AND ELECTROCATALYTIC CO2-TO-CO CONVERSION: FROM MOLECULAR DESIGN TO DEVICE INTEGRATION

17:20 – 18:30 **Poster Session II** (Poster no 22-42)

19:00 Conference Dinner

Augustiner Stammhaus, „weißer Saal“, Neuhauser Str. 27, München



Wednesday, November 11, 2026

Session 7 Chair: Anna Köhler (UBT)

09:00 **Emiliano Cortes** (LMU)

LIGHT, CHARGE, and ENERGY IN MOTION

09:20 **Johanna Eichhorn** (TUM)

INTERFACES, SURFACES, AND DEFECTS IN PHOTOELECTROCHEMICAL ENERGY MATERIALS

09:40 **Teresa Mauerer** (UBT)

HYDROPHILIC CROSSLINKED DIBENZOTHIOPHENE SULFOXIDE COPOLYMER FOR PHOTOCATALYTIC HYDROGEN EVOLUTION

10:00 **Lena Frank** (JMU)

π-STACKED RYLENE BISIMIDE ARRAYS AS FUNCTIONAL NANOSTRUCTURES FOR SINGLET FISSION

10:20 – 11:00 Coffee Break

Session 8 Chair: Frederic Laquai (LMU)

11:00 **Carolin Mueller** (FAU)

THE BRIDGE MATTERS: TD-DFT INSIGHTS INTO ALKYNE-BRIDGED DONOR-ACCEPTOR SYSTEMS

11:20 **Nivedita Pan** (LMU)

OPTICAL GAIN IN I-III-VI NANOCRYSTALS BEYOND BIEXCITONS

11:40 **Aimilios Christidis** (TUM)

ADVANCES IN THE SYNTHESIS OF INVERSE OPAL STRUCTURES FOR OXYGEN EVOLUTION REACTION

12:00 **Junior Wilfried Tadjeugue-Nangmo** (UBT)

MULTISCALE SIMULATION AND MACHINE-LEARNING SURROGATE OF CHARGE TRANSPORT ACROSS GRAIN BOUNDARIES IN ORGANIC THIN-FILM SEMICONDUCTORS

12:20 **Johannes Adelsperger** (JMU)

A TENSOR-PRODUCT FRAMEWORK FOR FRAGMENT-BASED CONFIGURATION INTERACTION: UNLOCKING COMPLEX BIEXCITONIC PATHWAYS IN MOLECULAR AGGREGATES

12:40 **Anna-Sophie Wollny** (FAU)

LONG- AND SHORT-RANGE ELECTRONIC COUPLING IN PARA VS. META CONJUGATION ON SINGLET FISSION

13:00 **Closing Remarks: Peter Müller-Buschbaum and Thomas Fässler** (TUM)

13:10-14:30 Snacks & Goodbye

List of Posters

Position	Name	Title
1	Ambasta	ADSORPTION-INDUCED STRUCTURAL AND OPTICAL CHANGES OF A THIOINDIGO-TYPE PHOTOSWITCH ON AU(111)
2	Amit	HAMILTONIAN LEARNING WITH GW-ACCURACY IN SOLIDS
3	Anjala	POLYELECTROLYTE-DIRECTED PLATINUM NANOSTRUCTURES FOR CATALYTIC APPLICATIONS
4	Baiju	HELICALLY CHIRAL ORGANOBORON COMPOUNDS: AZABOROLE- AND DIAZABOREPIN-TYPE-FUSED HELICAL SYSTEMS
5	Brand	TOWARDS SELF-CONSISTENT HUBBARD-CORRECTED DENSITY FUNCTIONAL THEORY
6	Christis	IMPROVING PHOTOELECTROCHEMICAL NITRATE REDUCTION ON COPPER OXIDE ELECTRODES
7	Darwish	STABILITY AND UNIFORMITY ENGINEERING IN PEROVSKITE NANOPARTICLES FOR ENHANCED PERFORMANCE
8	Dittloff	QUANTIFYING THERMAL, PHOTOVOLTAGE, AND DEFECT CONTRIBUTIONS TO TRANSIENT ABSORPTION OF TA_3N_5 PHOTOANODES
9	Färber	IMPACTING THE BALANCE BETWEEN CO_2 AND PROTON REDUCTION BY CONTROL OVER AGGREGATION IN A MODEL Π-CONJUGATED N-HETEROCYCLE – PROFLAVINE
10	Ganesan	INVESTIGATION OF SYMMETRY BREAKING CHARGE TRANSFER IN PHTHALOCYANINE DIMERS
11	Gareis	QUANTIFYING ELECTRON TRANSFER FLOWS WITH REAL-TIME DENSITY FUNCTIONAL THEORY
12	Garkusha	AZABOROLE-CONTAINING DIARYLETHENE PHOTOSWITCHES
13	Gindorf	PTHS: A POLYELECTROLYTE P3HT-DERIVATIVE FOR SEQUENTIALLY PROCESSED BILAYER OSCS
14	Goppelt	TOWARDS CD-SPECTROSCOPY OF SINGLE CHLOROSOMES
15	Graf	HOW TO FIX SILVER FOR PLASMONICS?
16	Griesbach	PHASE SEGREGATION IN MIXED HALIDE PEROVSKITES: RECONCILING MECHANISTIC AND THERMODYNAMIC MODELS
17	Gröninger	EXPLORING HETEROJUNCTIONS OF BI-FUNCTIONAL MATERIALS FOR NEW SOLAR BATTERY DESIGNS
18	Mariani	PLASMON-ASSISTED LITHIUM-IONS CAPTURE
19	Heilmaier	TRANSLATION OF COVALENT ORGANIC FRAMEWORK CATALYSTS FROM H-CELL TO FLOW CELL CONDITIONS FOR CO_2 ELECTROREDUCTION
20	Hilz	PORPHYRIN-FUSED HELICAL MULTILAYER NANOGRAPHENES
21	Hinrichs	CHIRAL N-ATOM DOPED NANOGRAPHENES
22	Hofbauer	ADVANCED SPECTROSCOPY AND EMISSION LINESHAPES: UNCOVERING EXCITONIC BEHAVIOR IN PEROVSKITES
23	Kavka	WHEN METALS BECOME MOLECULES
24	Kirchner	SINGLE-SITE WATER OXIDATION CATALYSIS WITHIN A HETEROGENOUS RUTHENIUM-CONTAINING ORGANIC FRAMEWORK
25	Kisker	INVESTIGATION OF COVALENT DONOR-ACCEPTOR PBI FOLDAMERS EMPLOYING VARIOUS SPACER MOIETIES

Position	Name	Title
26	Kunze	COMPOSITION TUNINING OF I-III-VI QUANTUM DOTS ENHANCES BAND-GAP EMISSION
27	Li	IN-SITU GISAXS STUDY OF FILM FORMATION IN LAYER-BY-LAYER PRINTED NON-FULLERENE ORGANIC SOLAR CELLS BASED ON GREEN SOLVENTS
28	Mack	CONTROLLING THE FLOW OF CHARGES ACROSS PHTHALOCYANINE@TRANSITION-METAL DICHALCOGENIDE INTERFACES
29	Gubanov	LANGMUIR–BLODGETT ASSEMBLY OF PM6 AND N2200 POLYMER PLANAR HETEROJUNCTIONS FOR INTERFACIAL PROBING
30	Moghimirad	PHOTOCATALYSIS WITH SELF-ASSEMBLED ORGANIC-INORGANIC HYBRID NANOSTRUCTURES
31	Narayanan	PHOTOLUMINESCENT CORE-SUBSTITUTED NAPHTHALENE BISIMIDE HETEROCYCLOPHANE WITH PLANAR CHIRALITY
32	Oberhofer	COMPUTATIONAL DESIGN OF A FERROELECTRIC FRAMEWORK MATERIAL BASED ON DIPOLAR ROTORS
33	Panagiotidis	IN SITU INVESTIGATION DURING SPUTTER DEPOSITION OF AG ON ZWITTERIONIC POLYMER FILMS
34	Pfaadt	SIDE-CHAIN AND IONIC FUNCTIONALIZATION OF N-TYPE CONJUGATED POLYMERS FOR OECT APPLICATIONS
35	Röhr	TOPOLOGY AS A DESIGN PRINCIPLE FOR MOLECULAR EXCITED STATES: FROM ROBUST EXCITONS TO ENTANGLED SPIN QUBITS
36	Schwanitz	TOWARDS AUTOMATED SPATIALLY RESOLVED CHARACTERIZATION OF ORGANIC SOLAR CELLS
37	Siebigs	TOWARDS SUBWAVELENGTH OLED PIXELS
38	Siegert	EXPLORING THE PHASE DIAGRAM OF FAPBI3 USING IN-SITU REFLECTANCE SPECTROSCOPY
39	Stickel	STRUCTURAL AND OPTICAL INFLUENCE OF LIGANDS ON PEROVSKITE QUANTUM DOTS
40	Wandke	OPTOIONIC EFFECTS IN NIOBATE-BASED ELECTRODE MATERIALS
41	Weiß	THROUGH-SPACE VERSUS THROUGH-BOND COUPLING: EFFECTS ON DOWN-CONVERSION IN [2.2]PARACYCLOPHANE LINKED TETRACENE OLIGOMERS
42	Werner	INSIGHTS INTO ELECTRON AND ENERGY TRANSFER IN TRANSITION METAL DONOR-ACCEPTOR SYSTEMS
43	Wilhelm	SECOND-SPHERE ENGINEERING OF IRON PORPHYRINS FOR ENHANCED CO_2 REDUCTION

TALKS

DESIGNING CONJUGATED POLYELECTROLYTES FOR OPTOELECTRONIC APPLICATIONS

Christopher Vogt[a], **Johannes C. Brendel**[a]

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Conjugated polyelectrolytes are crucial mixed ionic and electronic conductors that facilitate the coupling of aqueous ion penetration and electronic charge transport. This dual conductivity makes them highly effective as active layers in organic electrochemical transistors (OECTs), which are uniquely suited to bridging the gap between biological environments and solid-state electronics. Beyond bioelectronics, they also hold great potential for other possible applications, such as interface layers in organic hybrid solar cells or organic catalysts for water splitting [1]. However, optimising these materials requires navigating the complex structural trade-off between hydrophilicity, which enables rapid ion uptake, and well-ordered backbone chains, ensuring efficient electronic transport [2, 3].

This study presents a systematic approach to the design and synthesis of novel amphiphilic mixed-ion-electron-conducting polymers. Precursor polymers are prepared using controlled techniques such as Kumada catalyst transfer polymerisation (KCTP) or direct arylation polymerisation (DArP), and are then converted into the final conjugated polyelectrolytes. Precise side-chain engineering is employed to fine-tune the balance of hydrophilic and hydrophobic elements within active layers comprising donor backbones (e.g. thiophenes) or donor-acceptor copolymers containing diketopyrrolopyrrole (DPP). This is achieved by balancing oligoethylene glycol chains with alkyl spacers, or by varying the ionic groups. The resulting polymers are characterised using spectroscopic methods, including UV/Vis and ultraviolet photoelectron spectroscopy (UPS). Ultimately, these tailored materials are implemented as active layers in OECT devices to leverage their dual conducting properties, thereby establishing clear structure-property relationships to advance bioelectronic applications.

References

[1] L. Hu *et al.*, Macromolecules, 48, 5578-5586 (2015).
[2] Y. Wang, *et al*., Nat. Rev. Mater. 9, 249 (2024).
[3] H. Kim *et al.,* Adv. Sci. 11, 2306191 (2024).

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DISENTANGLING NONLINEAR SIGNAL ORDERS IN FLUORESCENCE-DETECTED MULTIDIMENSIONAL SPECTROSCOPY VIA INTENSITY CYCLING

Vishnu E. Krishnan[a], **Stefan Mueller**[a] **and Tobias Brixner**[a,b]

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Ultrafast spectroscopic measurements inherently include contributions from higher-order terms of the perturbation series, which can obscure the interpretation of nonlinear signals. Recently, our group demonstrated that intensity-dependent measurements (intensity cycling) enable the recovery of clean nonlinear responses in transient absorption [1] and coherently detected multidimensional spectroscopy [2]. Herein, we extend this method to fluorescence-detected multidimensional spectroscopy, using CdSe-based nanoplatelets as model samples, and successfully extract clean nonlinear signals.

References

[1] P. Malý *et al*, Nature 616, 280 (2023).

[2] J. J. Krich *et al*, J. Phys. Chem. Lett. 16, 5897 (2025).

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Perovskite Nanocrystal Hybrids as Tunable Platforms for Energy and Charge Transfer

Alejandro Cortés-Villena,[1,2] Alejandro Cadranel,[1,3,4] José Garcés-Garcés,[5] Alberto García-Ros,[5] Kobra Azizi,[6] Ángela Sastre-Santos,[5] Fernando Fernández-Lázaro,[5] Tomás Torres,[7,8] Julia Pérez-Prieto,[2] Raquel E. Galian[2], Dirk M. Guldi,[1]

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Controlling interfacial photophysics in perovskite nanocrystal (NC) hybrids is key to designing next-generation light-harvesting and energy-conversion systems. $CsPbBr_3$ NCs, with their tunable excitonic properties, are ideal donors for driving interfacial energy or charge transfer processes. Here, we present two complementary hybrid systems in which $CsPbBr_3$ NCs are interfaced with molecular acceptors to achieve unidirectional energy or charge transfer to surface-bound dyes.

In the first, $CsPbBr_3$ NCs coupled to carboxylated zinc phthalocyanines (ZnPc) undergo efficient Dexter-type singlet energy transfer, disaggregating the dye on the NC surface and enhancing its photophysics, despite new surface traps that partially reduce transfer efficiency. The resulting $CsPbBr_3$@ZnPc hybrid acts as an efficient photosensitizer, prolonging triplet lifetimes and generating singlet oxygen nearly quantitatively.

In the second, $CsPbBr_3$ NCs functionalized with perylenediimides (PDI) bearing phenyl or phenylpropyl spacers (NC@PDI-Ph, NC@PDI-PhPr) show not only spacer-dependent but also excitation-dependent dynamics, showing unidirectional electron transfer, and yielding extremely long-lived charge-separated states (34 and 63 μs, respectively).

Taken altogether, these results position perovskite NCs as versatile platforms for programming interfacial photophysics toward photocatalysis, energy harvesting, and optoelectronic applications.

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SHEDDING LIGHT ON WIDE-BANDGAP PEROVSKITES

Michael Saliba[a,b]

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Perovskite solar cells have come to the forefront of solar research in the last decade with certified efficiencies of now >26%. This is approaching rapidly the Shockley-Queisser limit for single-junction solar cells, implying that the main breakthroughs for perovskites were achieved with relatively narrow bandgaps.[1a,1b] Less progress, however, was made for wider bandgap perovskites, which are of interest for multijunction photovoltaics, detector applications, or water splitting. These wide bandgap perovskites are often comprised of fully inorganic components, which are hard to dissolve in conventional solvent systems and require more sophisticated synthesis as well as crystallisation techniques.

In this talk, I will discuss strategies to address these challenges by providing a library of hitherto unexplored wider bandgap perovskites using combinatorics. Mechanosynthesis is then studied to attain otherwise inaccessible liquid precursors permitting the realization, e.g., of “triple cation” wide bandgap perovskites.[2]

Unfortunately, the newly formulated liquid precursors often exhibit complex crystallization behaviour struggling to expel the typically used DMSO solvent. To delay the crystallization time, two strategies are proposed to remove the strongly complexating DMSO molecules through a) modified processing of the liquid thin-film[3] and b) a coordination solvent with a high donicity and a low vapor-pressure[4] leading to a marked improvement in the overall film quality.

Lastly, interface manipulation, especially on top of the formed perovskite, is becoming a central topic to advance further. Typically, this involves chemical surface treatments with a complex interaction. Here, light annealing is introduced as a universal, non-chemical approach to modify the perovskite surface resulting in a reduced surface recombination.[5]

References

[1a] Saliba et al. Energy & Environmental Science (2016), [1b] Turren-Cruz, Hagfeldt, Saliba; Science (2018)

[2] Ferdowsi,…, Saliba ; Chemistry of Materials (2021)

[3] Byranvand,…, Saliba; *One-Step Thermal Gradient-and Antisolvent-Free Crystallization of All-Inorganic Perovskites for Highly Efficient and Thermally Stable Solar Cells*, Advanced Science (2022)

[4] Zuo,…, Saliba; *Coordination Chemistry as a Universal Strategy for a Controlled Perovskite Crystallization*, Advanced Materials (2023)

[5] Kedia,…, Saliba; *Light Makes Right: Laser Polishing for Surface Modification of Perovskite Solar Cells*, ACS Energy Letters (2023)

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ALGORITHMS AND ANTISOLVENTS: THE ART OF BUILDING PERFECT 2D NANOPLATELETS

A.S. Urban[a]

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Two-dimensional perovskite nanoplatelets (NPLs) promise atomically precise emission control - but achieving that precision in the flask is anything but trivial. Their formation teeters on a fine balance between solvent polarity, precursor chemistry, and the split-second timing of an antisolvent drop. In this talk, I will show how data and diffraction together can turn this delicate art into a predictable science. Using in situ X-ray scattering and photoluminescence, we uncover how emissive nanocluster intermediates evolve into either rods or platelets depending solely on the antisolvent's dipole moment and hydrogen-bonding strength - essentially, how chemistry "decides" the dimensionality.[1] Building on this mechanistic insight, our machine-learning platform Synthesizer transforms these parameters into predictive maps of color, linewidth, and quantum yield.[2] Within just a few syntheses, it delivers nm-level precision over emission and aspect ratio, all under ambient conditions. Together, these studies define a quantitative recipe for crafting bright, narrow, and stable 2D NPLs - and hint at a future where algorithms, not trial-and-error, steer nanocrystal growth.

References

[1] K. Frank *et al*, Nature Communications. 15, 8952 (2024).
[2] N. A. Henke *et al*, Advanced Materials. 38, e09472 (2026).

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PREDICTING THE ELECTRONIC STRUCTURE OF HALIDE PEROVSKITE SURFACES AND NANOSTRUCTURES USING PHYSICS-INFORMED HAMILTONIAN LEARNING

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All-inorganic halide perovskites such as $CsPbBr_3$ are promising materials for next-generation optoelectronic and photovoltaic applications because of their tunable electronic structure, strong light absorption, and favorable charge-transport properties. However, their electronic behavior is strongly influenced by structural fluctuations, surface effects, and nanoscale confinement, requiring simulations of large atomistic systems under realistic finite-temperature conditions.

In this work, we investigate orthorhombic $CsPbBr_3$ in bulk, surface, and quantum-dot geometries using molecular dynamics simulations combined with HAMSTER [1], a physics-informed machine-learning framework for Hamiltonian prediction. HAMSTER enables efficient large-scale electronic-structure calculations by learning quantum-mechanical Hamiltonians from a limited number of first-principles calculations, thereby making simulations of extended molecular dynamics trajectories computationally feasible.

Electronic band structures and band gaps are calculated for finite-temperature molecular-dynamics snapshots to analyze the impact of dynamic disorder on the optoelectronic properties of $CsPbBr_3$. By comparing bulk, surface, and quantum-dot systems, we investigate how reduced dimensionality, surface-induced modifications, and quantum confinement influence the band-edge states and overall electronic structure. Particular attention is given to the relationship between atomic-scale structural fluctuations and electronic-property variations across different length scales.

Our results demonstrate that physics-informed Hamiltonian learning provides an efficient and accurate framework for studying temperature-dependent electronic properties of complex halide perovskites beyond the reach of conventional first-principles approaches. The present work further highlights the applicability of HAMSTER for understanding structural property relationships relevant to next-generation photovoltaic and optoelectronic devices.

References

[1] M. Schwade, S. Zhang, F. Vonhoff, F. P. Delgado & D. A. Egger, Nat. Commun. 17, 2652 (2026).

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ORGANIC MOLECULES FOR PHOTONIC AND QUANTUM TECHNOLOGIES

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Engineering the electronic energy landscape of organic light emitting molecules enables both enhanced device performance and entirely new functionalities. In particular, control of the triplet energies with respect to ground- and excited singlet states has allowed organic optoelectronic devices to overcome fundamental limitations imposed by spin statistics in electroluminescence. The ability to precisely design these states is opening new opportunities beyond conventional photonics, including the use of organic molecules as molecular color centers for quantum technologies.

In this presentation, I will introduce a novel concept that provides an alternative to thermally activated delayed fluorescence (TADF). By exploiting “hot” triplet states, this approach enables efficient conversion of non-emissive triplet excitons into emissive singlet states, thereby enhancing the luminescence efficiency of organic light-emitting diodes.

I will then introduce strategies for designing organic emitters with triplet ground states, establishing a platform for transferring concepts from solid-state color centers to molecular systems. Such molecular color centers combine the versatility of organic chemistry with functionalities traditionally associated with inorganic quantum materials.

Together, these developments illustrate how molecular-scale engineering can bridge photonics and quantum science, paving the way toward quantum bits based on individual organic molecules.

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CHIRAL BN-CONTAINING PAHS: FROM DESIGN AND SYNTHESIS TO FUNCTION

A. Nowak-Król[a]

[a]*University of Würzburg, Institute of Inorganic Chemistry and Institute for Sustainable Chemistry & Catalysis with Boron, Am Hubland, 97074 Würzburg, Germany*

The incorporation of boron and nitrogen into polycyclic aromatic hydrocarbons (PAHs) has become an established strategy for tuning their physical and optoelectronic properties. The most significant advances have been achieved in achiral compounds, leaving chiral boron-containing materials underexplored. Notably, less than a decade ago, only a handful of boron-containing helicenes had been reported [1-3]. In recent years, we have systematically expanded the family of BN-containing chiral materials, including single helicenes, multihelicenes, boron-containing photoswitches, and boron-centered spiro compounds [4-6]. The synthesis of some of these targets was challenging, with the introduction of boron, ligand exchange or the preparation of sophisticated precursors acting as bottlenecks.

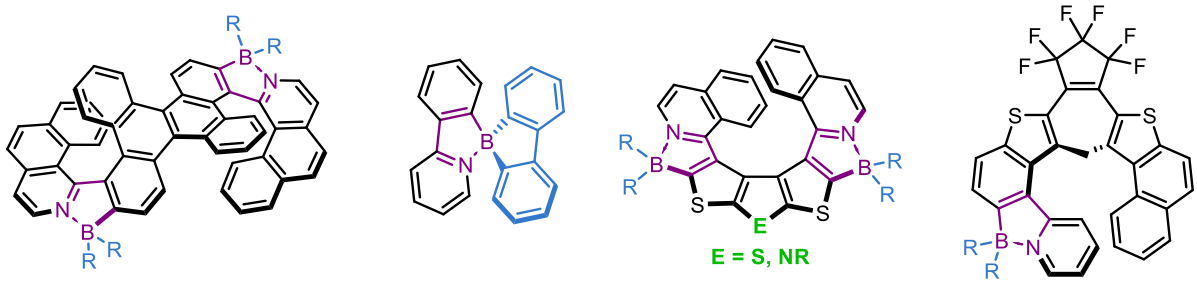


Figure 1. Molecular structures of selected BN-containing PAHs: multihelicenes, a boron-centered spiro compound, azaborahelicenes incorporating other main group elements and helically chiral photoswitches.

In this lecture, we will present selected boron-containing chiral compounds, e.g. π-extended helicenes containing multiple chiral axes and helicenes incorporating multiple heteroatoms. We will also discuss photochromic behavior of the first helical boron-containing photoswitches.

References

[1] A. Nowak-Król *et al.*, Chem. Sci. 15, 7408-7440 (2024).
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DISENTANGLING EXCITON DISSOCIATION PATHWAYS IN THE NON FULLERENE ACCEPTOR Y6

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The development of new materials for solar energy harvesting requires control of both molecular structure and intermolecular chromophore interactions. While interaction induced charge generation in single compounds has long been recognized, the unusually high yield of photogenerated charges in films of the non fullerene acceptor Y6 has renewed interest in its photophysics. I will show how optical signatures of interactions can be identified in absorption, photoluminescence and femtosecond transient absorption spectroscopy, and discuss the implications for interpreting charge generation models.[1]

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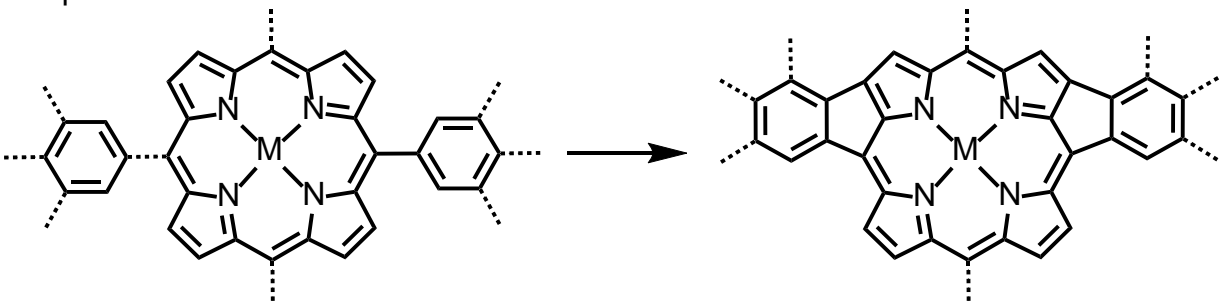
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ARYL-FUSED PORPHYRINS

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Fusing porphyrins to various polycyclic aromatic hydrocarbons is an excellent strategy to expand the π-system of porphyrins and add functionality. Thus, new chromophores are obtained which possess, among other interesting qualities, red-shifted UV/vis absorptions.



We present our approach to π-extended fused porphyrins via Scholl oxidation of meso-positioned aryl groups to the core.[1,2] Properties and interactions with fullerenes will be discussed.

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HOW COPPER OXIDATION IMPACTS THE INTERFACIAL pH AND THEREBY STEERS PRODUCT SELECTIVITY IN PULSED CO_2 REDUCTION ON COPPER ELECTRODES

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Pulsed electroreduction of CO_2 on Cu electrodes is known to substantially suppress the competing H_2 evolution reaction, produce morphological restructuring and stabilize product selectivities and efficiencies [1,2]. In this contribution, we investigate the impact of the upper recovery pulse potential E_u on Faradaic efficiencies, surface morphology, cyclic voltammetry and open circuit potential transients. All measurements were carried out on mechanically polished polycrystalline Cu disk electrodes in CO_2-saturated 100 mM $KHCO_3$, with the reactive pulse potential kept at $E_l = -1.15\ V_{RHE}$.

We find that there is a threshold upper pulse potential E_{th} that marks a transition from a monotonic decrease in H_2 evolution with increasing E_u to a product composition that is nearly independent of E_u. Furthermore, we show that, for values of E_u below E_{th}, the open circuit potential tracks the interfacial pH. This allows us to draw conclusions about the pH profile between interface and bulk electrolyte: below E_{th} the interfacial pH is always larger than the bulk pH and the profile changes in a complicated manner over extended pulsing times. For values of E_u above this threshold, the recovery pulse restores the bulk pH at the surface and leads to a vanishing pH gradient into the bulk in the order of a second.

The driving force for adjusting the pH is Cu oxidation to Cu(I) and / or Cu(II) species. This interpretation is supported by cyclic voltammetry, morphology measurements, and selectivity maps for various pulse lengths and time ratios between reactive and recovery phase for $E_u > E_{th}$.

To provide direct experimental evidence for this process, an in situ bipotentiostatic approach was developed to quantify the interfacial pH. The setup employs a gold microelectrode functionalized with a 4-nitrothiophenol (4-NTP) derived self-assembled monolayer [3]. A temporal resolution of <200 ms enables the accurate tracking of pH transients during single pulse cycles. Coupled with a precision stepper motor for controlled spatial positioning, this technique allows for the complete profiling of the pH gradient across the boundary layer.

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GOOD VIBRATIONS: OPTOP-STRUCTURAL CONTROL OF FUNCTIONAL MATERIALS

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Ultrafast all-optical control over the properties and functionalities of molecules and materials is desirable, with prominent examples in femtochemistry or light-induced phase transitions. Femtosecond light pulses can drive electronic excitations, enabling access to transient nonequilibrium states and revealing pathways of energy relaxation. In contrast, direct optical control of structural degrees of freedom offers a complementary yet comparatively underexplored route to material manipulation.

Here, we present recent progress in exploiting optically-driven coherent lattice motion as an active handle to tailor material properties on femtosecond timescales. Using structure-sensitive ultrafast electron diffraction and all-optical spectroscopy, we demonstrate that tailored light fields selectively excite key vibrational modes to control the efficiency of metal-insulator transitions, manipulate nanoscale domains below the diffraction limit, and steer ferroic order and topology. Such opto-structural control represents a versatile pathway for ultrafast materials engineering. We conclude with an outlook on extending these concepts to light-harvesting molecular systems, where selective vibrational excitation may enable new strategies for controlling energy flow and functionality.

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TIME-RESOLVED FLUORESCENCE SPECTROSCOPY FOR RESEARCH ON SOLAR TECHNOLOGIES: A KEYLAB APPROACH

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Advancing next-generation solar technologies requires a detailed understanding of photophysical processes across a wide range of material systems. Addressing these challenges demands interdisciplinary approaches that combine advanced experimental techniques with specialized knowledge in materials synthesis, characterization, and theory. However, in spectroscopy, researchers often face challenges due to restricted access to specialized instrumentation and the expertise required to design and interpret sophisticated spectroscopic experiments.

To overcome these barriers, the Bayreuth Institute for Macromolecular Research (BIMF) provides access to state-of-the-art optical spectroscopy infrastructure through the KeyLab for Optical Spectroscopy within the Bavarian Polymer Institute (BPI). The KeyLab bridges method development and user-oriented applications by integrating commercial and custom-built instrumentation within a modular and adaptable framework. Fluorescence lifetime, fluorescence correlation, and single-molecule spectroscopy techniques enable investigations of photophysical processes across a wide range of temporal and spatial scales. These capabilities are complemented by a highly flexible custom-built platform with cryogenic operation, allowing tailored studies under diverse experimental conditions. Together, these approaches extend beyond conventional absorption and emission spectroscopy, providing powerful tools to investigate exciton dynamics, energy transfer, charge-carrier interactions, and structure–property relationships in materials relevant to solar-energy conversion.

The KeyLab has supported studies ranging from optical-property mapping in hybrid perovskite materials to investigations of individual photosynthetic antenna complexes, demonstrating its applicability across both synthetic and biological light-harvesting systems. By lowering technical barriers and fostering interdisciplinary collaboration, the KeyLab enables researchers from diverse fields to address fundamental questions in solar-energy conversion and related areas using advanced optical spectroscopy methods.

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PHASE SEGREGATION IN MIXED HALIDE PEROVSKITES: RECONCILING MECHANISTIC AND THERMODYNAMIC MODELS

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Mixed halide perovskites have emerged as leading contenders for multi-junction solar cells due to their tunable band gaps, controlled by halide composition, and excellent optoelectronic properties. However, compounds such as $MAPbI_{3-x}Br_x$, suffer from light-induced halide segregation, resulting in compositional heterogeneity that degrades device performance.

Despite extensive experimental and theoretical efforts, the physical origin of light-induced halide segregation in mixed-halide perovskites remains debated. Several driving forces have been proposed, including polaronic strain [1], band-gap-driven carrier stabilization [2], internal electric fields [3], and photo-induced redox processes [4]. While each model captures specific aspects of the phenomenon, seemingly similar experimental observations are often interpreted differently across the literature.

We compare the underlying assumptions, predictions, and experimental signatures of these models and argue that many apparent inconsistencies arise from insufficient separation of kinetic and thermodynamic aspects. Specifically, the segregation rate is largely governed by halide migration kinetics, whereas the final extent of segregation is determined by the underlying free-energy landscape. [5]

We propose that the latter can be described within a generalized thermodynamic framework, in which different microscopic models correspond to different ways of modifying the free-energy balance under illumination. The separation of kinetic and thermodynamic aspects provides a basis for more comparable experimental studies. Building on this, we employ targeted investigations on mixed cation systems and tailored additives to distinguish between contemporary models and elucidate the physical origins of halide segregation.

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LENGTH-DEPENDENT OPTOELECTRONIC BEHAVIOUR IN NANOGRAPHENES

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Molecular nanographenes are emerging as promising materials for optoelectronic and energy-related applications due to their unique and tuneable optoelectronic properties.[1] While significant advances have been made over the past decade in the synthesis of atomically precise nanographenes, a comprehensive understanding of their photophysical and electrochemical behaviour remains in its early stages.[2,3] In this work, we present a systematic photophysical investigation of a series of molecular nanographenes with varying lengths.[4,5,6] Furthermore, we explore their interactions with porphyrins and study their behaviour in the aggregated state using a broad range of ultrafast spectroscopic techniques.

Interestingly, we found that increasing the nanographene length results in an energetic proximity between the S_1 and S_2 states, giving rise to a rarely observed anti-Kasha fluorescence. This is accompanied by strong vibronic coupling, which leads to deviations from the widely used Franck–Condon approximation, in favour of Herzberg-Teller activities. The nanographene length also influences the excited-state deactivation pathways in their porphyrin hybrids, as revealed by ultrafast transient absorption spectroscopy. Notably, the larger nanographene-porphyrin hibrid exhibits a “ping-pong” energy transfer mechanism, where energy is transferred from the nanographene to the porphyrin and then back again.

Furthermore, the self-assembly behaviour of these compounds in solution was examined in detail, revealing the formation of dimers followed by two-dimensional supramolecular polymers. Exciton and charge carrier dynamics within these structures were probed using transient emission microscopy and ultrafast terahertz spectroscopy. Our findings provide a deeper understanding of the optoelectronic properties of nanographenes and underscore the potential of such assemblies for applications in organic electronics, including solar cells and field-effect transistors.

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ANISOTROPIC EXCITON DIFFUSION IN ORGANIC SINGLE-CRYSTAL MATERIALS

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The exciton diffusion length is one of the key figures of the energy conversion material and a major bottleneck in optoelectronic applications [1]. Here we employ confocal laser scanning microscopy combined with time-correlated single photon counting (TCSPC) to map exciton transport in space and time [2]. Pulsed excitation laser is focused onto the sample, while the photoluminescence is collected from a laterally displaced position through an independently scanned detection path.

Applying this approach to single crystals of an n-butyl-substituted naphthalenediimide–bithiophene (NDI-T2) derivative, we observe a pronounced anisotropy: revealing different diffusion lengths along orthogonal crystal orientations, with an additional dependence on the excitation polarization set by a half-wave plate. This suggests that exciton diffusion is governed by the crystal packing along two orthogonal directions: the transition dipole is oriented along the molecular long axis, while excitons migrate preferentially along the π–π stacking direction.

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PHYSICS-INFORMED HAMILTONIAN LEARNING FOR PEROVSKITE ELECTRONIC STRUCTURE WITH HAMSTER

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Understanding the electronic structure of functional materials is essential for connecting atomic structure to optoelectronic behavior. This is particularly important in halide perovskites, where soft lattice dynamics and temperature-driven structural fluctuations give rise to unusual electronic properties relevant for solar cells, light-emitting devices, and other energy technologies. However, resolving these effects with conventional computational methods such as density functional theory remains computationally demanding, especially when finite-temperature sampling or complex chemical compositions are required.

Recent advances in deep neural network approaches offer a promising route to efficiently predict accurate effective Hamiltonians. However, incorporating temperature-dependent effects remains challenging, largely because finite-temperature lattice dynamics typically require a substantial amount of training data. In this work, we present HAMSTER [1] (Hamiltonian-learning Approach for Multiscale Simulations using a Transferable and Efficient Representation), a physics-informed machine-learning framework designed to construct accurate effective electronic Hamiltonians with reduced training-data requirements.

We apply this approach to halide perovskites to investigate how structural changes modify their electronic structure, with particular focus on the band gap. In this way, HAMSTER goes beyond efficient prediction of electronic properties by providing a chemically interpretable picture of how structural distortions and bonding changes shape the electronic response of soft perovskites.

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PHOTOFUNCTIONAL CONTROL OF CYCLOPHANES VIA HOST-GUEST COMPLEXATION

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Nature discloses principles of solar energy conversion. Among those are light harvesting and energy transfer, the creation of long-lived excited and charge-separated states and the tuning of dye-dye interactions as exemplified by the “special pair” of two (bacterio-)chlorophyll dyes at the core of the photosynthetic reaction center.
Motivated by these photofunctional dimers, we recently synthesized cyclophanes composed of terrylene bisimides (TBI)[1] and coronene bisimides (CBI)[2], whose photofunctional properties can be tuned through the encapsulation of guest molecules. The π-π and C-H-π interactions between the cyclophane host and large planar aromatic guests can activate and modulate excited-state pathways involving both singlet and triplet manifold, leading to photophysical processes and long-lived excited states that are not observed in the isolated cyclophane. These studies establish a versatile approach for sophisticated control of photofunctional properties in host-guest systems as demonstrated by a variety of recent examples from our laboratory.[3]

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A SIMPLE PHYSICAL MODEL FOR CHEMICAL CONTROL OF DISORDER AND DYNAMICS IN HYBRID PEROVSKITE ENERGY MATERIALS

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Solution-processable hybrid organic–inorganic metal halides which adopt the perovskite crystal structure have demonstrated unexpected performance in electronics [1,2], solar cells [3], radiation detectors [4], and light emitters [5]. However, instability, structural disorder, and dynamic disorder pose ongoing performance and reliability challenges, hindering the application of these materials [6,7].

Compared to the long-studied and diverse family of perovskite oxides, these heavy halides accommodate a different and narrower set of ions by virtue of the large size and monovalent charge of the halides, even incorporating small organic molecular cations on the larger cation site. Such molecular cations exhibit lower symmetry than the usual monatomic ones, introducing orientational degrees of freedom [8,9] and anisotropic steric and hydrogen-bonding interactions that are not present in oxide analogs [10].

Inspired by the successes of statistical physics models for oxide ferroelectrics and dielectrics [11,12] and elastic multipole expansions for describing anisotropic defects [13], we developed a microscopic effective Hamiltonian designed to capture the essential interactions in many hybrid perovskites. This model reproduces key experimental observations, exhibits intriguing properties related to geometric frustration, and allows us to predict new superlattice alloy compositions which may exhibit enhanced thermodynamic stability and suppressed disorder and carrier–phonon scattering.

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PEROVSKITE TANDEM SOLAR CELLS: FROM EFFICIENCY TO STABILITY

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The continued reduction in photovoltaic electricity costs strongly depends on increasing the power conversion efficiency of solar cells per unit area. Tandem solar cells, which combine photoactive materials with complementary bandgaps, provide a promising pathway to surpass the efficiency limits of single-junction technologies by utilizing a broader portion of the solar spectrum. Among these, perovskite/silicon and all-perovskite tandem solar cells have emerged as leading candidates due to their outstanding optoelectronic properties and fabrication versatility. However, achieving both high efficiency and long-term operational stability remains a major challenge.

In this talk, I will present our efforts toward developing efficient and stable perovskite-based tandem solar cells by investigating voltage losses and degradation mechanisms under operating conditions. In particular, I will focus on imaging voltage-losses and probing phase and interphase instabilities across perovskites with different bandgaps.

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ALKALI AND SCN^- ADDITIVE ENGINEERING FOR ENHANCED LATTICE STABILITY IN WIDE-BANDGAP INVERTED PEROVSKITE SOLAR CELLS

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Inverted (p–i–n) perovskite solar cells based on a wide-bandgap (~1.77 eV) absorber were fabricated with alkali metal ions (e.g., K^+,Cs^+, Rb^+) as cation additives and SCN^- as an anion additive, and their roles in the perovskite lattice and influence on device performance were investigated. The additives are found to affect crystallization behavior and lattice structure, with evidence suggesting partial incorporation into the lattice or occupation of vacancy sites, contributing to reduced defect density and suppressed non-radiative recombination. Under operando illumination conditions, the modified films exhibit improved structural and optoelectronic stability, indicating that the combined additive strategy mitigates ion migration and enhances resistance to light-induced degradation. These results highlight the interplay between additive chemistry and lattice dynamics in wide-bandgap perovskites and provide a practical pathway toward more stable and efficient inverted perovskite solar cells.

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SCALABLE INKJET-PRINTED PEROVSKITE/SILICON TANDEM SOLAR CELLS VIA HYBRID TWO-STEP DEPOSITION

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Metal-halide perovskites are promising wide-bandgap absorbers for tandem photovoltaics, but industrial deployment requires scalable, conformal coating over textured silicon. Hybrid two-step deposition addresses this challenge: inorganic precursors are thermally evaporated to cover the silicon texture, followed by solution deposition of organic precursors to promote intermixing and crystallization. As the second step, we use inkjet printing as a precise and scalable method.

We investigate the interaction between vapor-deposited inorganic scaffolds and picoliter-sized inkjet droplets, and optimize the precursor morphology. The resulting hybrid two-step inkjet-printed perovskite solar cells achieve a power conversion efficiency (PCE) above 18%. Extending the process to wide-bandgap absorbers with effective surface passivation yields single-junction devices with PCE above 20%. Transferring the process to industrially textured silicon enables the first perovskite/silicon tandem cells fabricated by hybrid two-step inkjet printing, reaching 27.4% PCE.

For fully scalable fabrication, dip-coating is introduced to deposit the perovskite interfacial layers. A mini-module with more than 100 times the active area of the cell shows minimal upscaling losses and reaches 17.8% PCE. Applied to small-textured silicon, the process exceeds 30% PCE in hybrid two-step inkjet-printed tandems. Inkjet printing also provides the deposition precision required at substrate edges, where other liquid coating methods face challenges.

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UPSCALLING OF FLEXIBLE PEROVSKITE SOLAR MODULES

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Flexible perovskite solar modules (f-PSMs) have emerged as promising candidates for lightweight and portable photovoltaic applications. However, bridging the gap between laboratory-scale devices and industrial-scale manufacturing remains challenging due to difficulties in achieving uniform large-area film formation, efficient charge extraction, long-term operational stability, and mechanical durability under scalable processing conditions. In this work, we present a comprehensive strategy for upscaling flexible perovskite modules based on scalable interface engineering and roll-to-roll (R2R)-compatible fabrication approaches.

First, molecularly engineered electron transport layers based on self-assembled fullerene phosphonic acid interlayers are developed to improve charge extraction and device reliability in fully printed flexible devices. Second, a simplified dual-interface design is demonstrated, where multifunctional molecular interlayers simultaneously regulate both electron- and hole-selective contacts, reducing device complexity while maintaining high photovoltaic performance. Third, a vapor-phase thiol treatment is integrated into an R2R-relevant manufacturing route to control perovskite crystallization, suppress defects, and enhance fracture resistance through grain-boundary anchoring. This approach enables exceptional mechanical robustness, retaining over 90% of the initial performance after 25,000 bending cycles.[1,2,3]

By combining scalable transport-layer engineering, interfacial defect passivation, and vapor-phase crystallization control, flexible perovskite modules with high efficiency, excellent operational stability, and outstanding mechanical durability are achieved. This work highlights a pathway toward translating perovskite photovoltaics from laboratory-scale demonstrations to industrially relevant large-area manufacturing.

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SINGLE-METAL-SITES IN COFS FOR PHOTO- AND ELECTROCATALYTIC CO_2-TO-CO CONVERSION: FROM MOLECULAR DESIGN TO DEVICE INTEGRATION

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A Molecular fac-[M(CO)3(NN)X] complexes (M = Re, Mn; NN = bipyridine or phenanthroline derivatives) are among the most selective catalysts for the reduction of CO_2 to CO, but their operational lifetime in solution is fundamentally limited by bimolecular deactivation pathways. Covalent Organic Frameworks (COFs) offer a way to combine the precision of molecular catalyst design with the robustness of a heterogeneous, crystalline scaffold: their modular building blocks provide well-defined coordination pockets that immobilize single metal sites at predictable positions within an ordered, porous lattice.

This talk presents a series of imine-linked 2D COFs in which the metal-binding linker (bipyridine or phenanthroline) and the structure-directing node (dibenzochrysene, pyrene) were rationally varied to tune crystallinity, stacking, porosity and the electronic coupling between framework and metal center.

Powder X-ray diffraction combined with STEM-HAADF imaging allowed the atomistic-level distribution of metal sites within the COF lattice to be resolved, establishing genuine single-site character. Systematic variation of the metal loading reveals structure-activity relationships linking site occupancy, interlayer stacking rearrangements and photocatalytic performance, while in-situ FTIR spectroelectrochemistry connects the immobilized catalytic cycle to that of the parent molecular complex.[1] Under illumination, the resulting Re-COFs sustain CO evolution for tens of hours exceeding their molecular analogues.[2]

Moving from photocatalysis toward application, a Mn-functionalized phenanthroline-COF is integrated as the active layer of a gas-diffusion electrode in a catholyte-free, zero-gap membrane-electrode-assembly electrolyzer, where the framework suppresses Mn^0–Mn^0 dimer formation and sustains high partial current densities for CO_2-to-CO conversion.[3] Together, these results outline a design logic that carries single-metal-site catalysis from molecular blueprint to structurally resolved hybrid photocatalysts and, ultimately, to industry-relevant electrocatalytic devices.

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LIGHT, CHARGE, AND ENERGY IN MOTION

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Understanding and controlling energy flow at the nanoscale is essential for designing materials that harvest light, drive chemical reactions, and store energy efficiently. Our research combines nanophotonic materials design with advanced imaging and spectroscopy methods to reveal how energy and charge move across diverse functional nanomaterials [1–10].

This work explores plasmonic, photonic, and photocatalytic systems that convert light into chemical bonds, with a focus on solar-driven H_2 evolution and CO_2 reduction. Through tailored nanostructure design, we uncover fundamental mechanisms and establish principles for efficient and scalable energy conversion.

We also develop imaging and characterization platforms that visualize charge and energy dynamics in real time and with nanometric precision. These approaches extend beyond nanophotonics to catalytic, light-emitting, battery, and 2D materials, enabling imaging-guided optimization of material function.

Together, this integrated strategy links material design, energy dynamics, and reactivity to advance the visualization, control, and optimization of energy flow from the nanoscale to practical applications.

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INTERFACES, SURFACES, AND DEFECTS IN PHOTOELECTROCHEMICAL ENERGY MATERIALS

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Transition-metal oxide and nitride semiconductors offer considerable promise for photoelectrochemical (PEC) energy conversion. Yet their efficiency and stability are often limited by surface and interface processes, where atomic structure, electronic defects, and chemical reactions are strongly coupled. In such systems, disorder, point defects, and dynamic surface transformations govern charge transport, interfacial charge transfer, and degradation. Here, we investigate Ta_3N_5 thin film photoanodes as a model system to determine how defect chemistry, structural disorder, and surface composition influence photoelectrochemical performance and stability.

Using controlled synthesis from different precursors, we prepared Ta_3N_5 photoelectrodes with varied oxygen contents, structural order, and shallow- and deep-level defect concentrations. Reduced oxygen incorporation improves long-range structural order but increases deep-level defect densities, whereas higher oxygen concentrations introduce shallow donor states and passivate detrimental mid-gap defects. Depth-sensitive characterization reveals oxygen-enriched, structurally disordered surface regions with elevated defect densities relative to the bulk. The extent and nature of these surface layers depend strongly on precursor chemistry: Ta_3N_5 derived from tantalum oxide forms an extended amorphous oxide-rich surface, while Ta_3N_5 from tantalum nitride or tantalum exhibits thinner, more crystalline surface regions.

Photoelectrochemical stability measurements show that under water oxidation conditions, Ta_3N_5 photoanodes degrade via the formation of a surface oxide layer that suppresses hole injection and enhances recombination. In contrast, under ferrocyanide oxidation conditions, oxygen-rich films exhibit improved long-term stability, whereas oxygen-poor films with high deep-level defect densities degrade rapidly. Specifically, shallow oxygen donors can kinetically stabilize the interface, whereas deep-level defects facilitate rapid photocarrier trapping and surface oxidation. Brief hydrofluoric acid treatment removes the disordered surface layer, improves crystallinity and hydrophilicity, and enhances performance and stability. Overall, this work highlights the importance of defect, surface, and interface engineering for stable and durable photoelectrodes.

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HYDROPHILIC CROSSLINKED DIBENZOTHIOPHENE SULFOXIDE COPOLYMER FOR PHOTOCATALYTIC HYDROGEN EVOLUTION

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Photocatalytic hydrogen evolution with organic semiconductors and conjugated polymer semiconductors is a growing research field as they allow facile synthetic modifications. A well-known linear polymer photocatalyst is the homopolymer of dibenzothiophene sulfoxide (DBTO), as well as its copolymers with phenylene and fluorene.[1] The inherent hydrophobicity of conjugated polymers remains a key bottleneck for wettability and thus photocatalytic applications. To address this limitation, hydrophilic segments are introduced as sidechains.[2,3] They enhance the polymer/water interface, the solubility, and the conductivity.[3] Additionally, crosslinking the linear polymers with hydrophilic segments enhances the hydrogen evolution activity in comparison to aliphatic side chains.[2]

Here, we will present the synthesis of a crosslinked, hydrophilic copolymer P(DBTO-TeEG-Ph) of the DBTO unit and phenylene. Bis(1,4-dibromobenzene) units are linked with a tetraethylene glycol side chain. Subsequent Suzuki-Miyaura cross polymerisation formed the crosslinked polymer P(DBTO-TeEG-Ph). The resulting polymer was thoroughly characterised for its structural and optical properties. The amount of residual Palladium, that can act as a cocatalyst in hydrogen evolution reaction (HER), was found to be low. Contact angle measurements confirmed the hydrophilic nature of the surface with contact angles below 90°. Physisorption experiments showed that the polymer has a non-porous structure.

HER experiments using a sun simulator with a cut-off (λ> 420 nm) filter without cocatalyst addition in a 1:1:1 mixture of water, triethylamine and methanol exhibited a higher activity compared to the non-crosslinked polymer and the hydrophobic linear polymer, as well as comparable literature networks.[1,2,4] Addition of 1 wt% of Platinum as cocatalyst increases the H_2 activity further.

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π-STACKED RYLENE BISIMIDE ARRAYS AS FUNCTIONAL NANOSTRUCTURES FOR SINGLET FISSION

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The photophysical phenomenon of singlet fission (SF) has the potential to overcome the Shockley-Queisser limit for single-junction solar cells by enabling the absorption of high-energy photons without energy loss. SF is an energy conversion process whereby a singlet exciton is split into two triplet excitons via an intermediate multiexciton state.[1] In recent years, the ability of perylene and terrylene bisimide (PBI and TBI) dyes to promote SF has been intensely studied especially with regard of the present Coulomb and charge-transfer (CT) couplings and their influence on the observed optical properties.[2–4]

Herein, we report the synthesis and investigation of co-facially slip stacked PBI-TBI arrays consisting of PBI cores of varying length substituted with TBI moieties at the outer positions. The covalent attachment of the monomers enables precise control of the structural arrangement and thus, of the Coulomb and CT couplings which were investigated using time-dependent DFT calculations. Steady-state absorption and emission, as well as time-resolved absorption and photoluminescence measurements were performed to gain insights into the photophysical processes. The efficiency of the formation of the multiexciton state was found to depend on the length of the PBI-TBI stacks, indicating varying mechanisms of the SF process.

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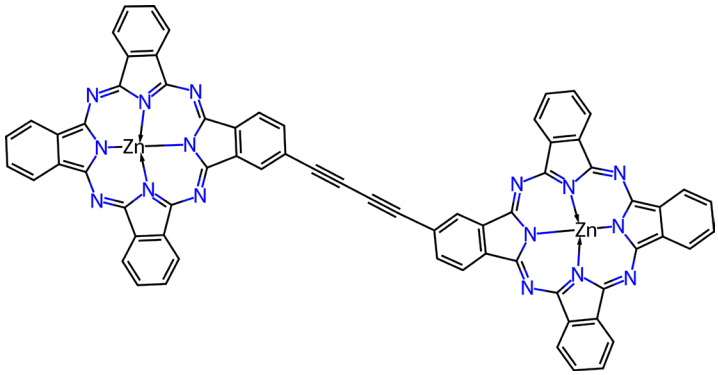
THE BRIDGE MATTERS: TD-DFT INSIGHTS INTO ALKYNE-BRIDGED DONOR-ACCEPTOR SYSTEMS

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Light-induced charge and energy transfer processes in donor-acceptor molecular systems are central to the design of functional materials for artificial photosynthesis, photocatalysis, and molecular optoelectronics [1]. In particular, zinc complexes provide a versatile platform for investigating how molecular architecture governs excited-state properties. In this contribution, we present a comparative computational study of two classes of zinc-complex based donor-acceptor systems designed to elucidate the influence of alkyne bridges on electronic structure and excited-state spectroscopy.

The first class comprises zinc porphyrins functionalized with anthracene and dimethylaminophenyl donor groups, with and without an ethynyl linker, while the second consists of zinc-porphyrin dyads connected through monoethynyl or butadiynyl bridges. Using DFT and TD-DFT calculations, we identify the electronic configurations underlying the transient absorption response and establish structure-property relationships that enable the assignment of experimentally observed spectral features to specific excited-state species. Our results reveal how alkyne bridges modulate electronic coupling and excited-state localization, providing molecular-level insight into the transient spectroscopic signatures of zinc-porphyrin donor-acceptor assemblies.



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Optical gain in I-III-VI nanocrystals: Involvement of non-bandgap excitons

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Optical gain has been thoroughly studied in a variety of colloidal II–VI and IV–VI nanocrystals (NCs) that contain toxic heavy metals, with the gain mechanism largely attributed to band-gap biexcitons. Finding suitable eco-friendly material for light amplification, however, remains a challenge. Recently, in our group, $AgInS_2$ NCs have been synthesized with excellent band-gap emission rather than defect-related emission [1,2]. Here, we report the first observation of amplified spontaneous emission (ASE) and optical gain in $AgInS_2$ NCs. Interestingly, the ASE peak appears almost at the center of the PL spectrum (see Fig. 1), a behavior not previously observed in NCs [3]. We argue that the gain in these NCs involves a higher-lying exciton with a larger oscillator strength and enables light amplification by overcoming the limitation of the lower oscillator strength of the band-gap exciton. The comparison of the optical gain duration with the biexcitonic and multiexcitonic lifetimes obtained from pump-fluence-dependent transient absorption measurements support our conclusions. The experimentally determined threshold and gain coefficient values indicate the feasibility of using these materials in future eco-friendly quantum dot lasers [4].

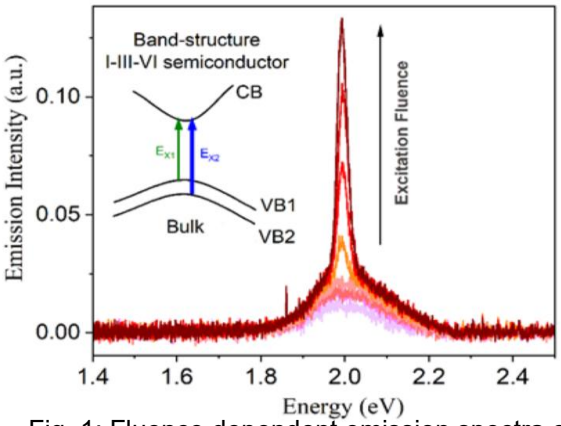


Fig. 1: Fluence dependent emission spectra of $AgInS_2$ NCs film. The inset shows the band structure.

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ADVANCES IN THE SYNTHESIS OF INVERSE OPAL STRUCTURES FOR OXYGEN EVOLUTION REACTION

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The development of oxygen evolution reaction (OER) catalysts in alkaline media from intermetallic alloys such as NiGe, and the recent clathrate $Ba_8Ni_6Ge_{40}$, inspired our interest in transferring these ideas to well-defined nanostructured materials.[1,2] Several years ago, we developed a synthetic route by infiltrating polymethyl methacrylate opals with diameters between 250 and 300 nm with reactive, soluble intermetallic precursors comprising $[Ge_9]^{4-}$ clusters.[3] Here, we report a variation of the synthetic protocol in which "KGeP" and "$K_{12}CoGe_{17}$" are dissolved in LiCl and mixed with the transition-metal complex $Ni(CO)_2(PPh_3)_2$ to form ternary Ni-Ge-P and binary Ni-Ge inverse opal thin films (see Figure 1b and 1c). The catalytic performance of these films for OER is tested on fluorine-doped tin oxide and nickel foam substrates.

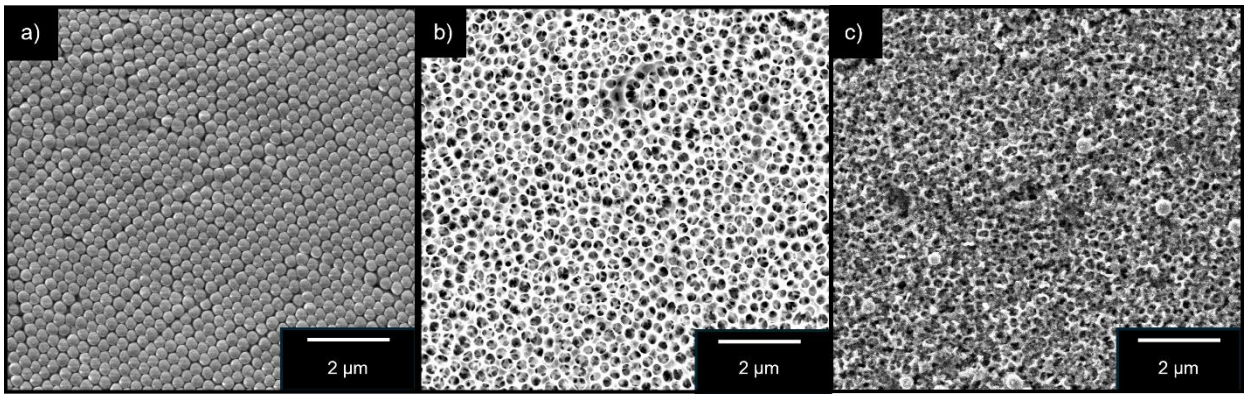


Figure 1: Scanning Electron Microscopy micrographs of: a) PMMA opals on FTO, b) Ni-Ge-P inverse opals, c) Ni-Ge inverse opals

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MULTISCALE SIMULATION AND MACHINE-LEARNING SURROGATE OF CHARGE TRANSPORT ACROSS GRAIN BOUNDARIES IN ORGANIC THIN-FILM SEMICONDUCTORS

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Charge-carrier mobility in polycrystalline organic thin films is typically orders of magnitude below single-crystal values, with grain boundaries (GBs) the dominant transport bottleneck. We present a multiscale framework linking thin-film morphology to device-level mobility in perylene derrivatives-based semiconductors (Figure 1). Molecular packings are draw both from experimentally resolved crystal structures and from numerical prediction, the latter used to explore newly designed high-mobility organic semiconductors. Realistic GB networks are generated by anisotropic phase-field growth simulations, reproducing experimentally relevant polycrystalline film morphology.

The local electronic structure is computed from first principles to evaluate the charge-carrier mobility [1], with explicit thermal fluctuations captured by molecular-dynamics sampling of the dynamic disorder. Boundaries that disrupt the molecular arrangment introduce deep traps and suppressed coupings, while electrostatic disorder broadens the site-energy distribution, substantially reducing the effective mobility.

To render the worflow manageable across the entire GB networks and chemical design space, we develop a machine-learning surrogate that infers the transport parameters dorectly from the local molecular packing, facilitating efficient high-throughput screening.

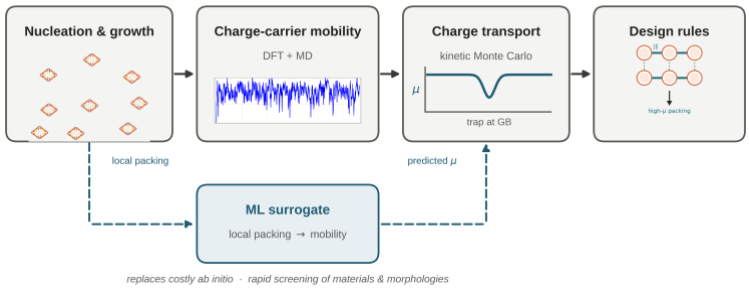


Figure 1. Multiscale workflow.

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A TENSOR-PRODUCT FRAMEWORK FOR FRAGMENT-BASED CONFIGURATION INTERACTION: UNLOCKING COMPLEX BIEXCITONIC PATHWAYS IN MOLECULAR AGGREGATES

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Biexcitonic states govern critical photophysical processes ranging from singlet fission to exciton-exciton annihilation. Understanding these mechanisms requires treating a diverse manifold of two-particle states, including localized Frenkel pairs, charge-transfer biexcitons, and highly correlated triplet pairs, on equal footing. In our recent work [1], we demonstrated that mixed configurations featuring both localized and charge-transfer character act as essential electronic gateways that bridge the single- and multi-exciton manifolds. However, mapping these interconnected pathways in extended molecular materials pushes traditional quantum chemical methods to their limits, necessitating a scalable approach that preserves clear physical interpretability.

To enable more advanced multiexciton studies, we present a rigorously reformulated fragment-based configuration interaction methodology. Rather than relying on global determinant expansions, this approach constructs the supermolecular diabatic basis through the restricted tensor products of isolated, aggregate aware optimized adiabatic fragment states. Inter-fragment couplings are evaluated by taking the tensor products of local transition density matrices, governed by a modified fermionic scattering logic that strictly enforces Pauli anti-symmetry. To restore rotational invariance, the basis is spin-adapted via genealogical coupling pathways. Finally, instead of a brute-force full diagonalization, the framework employs a targeted group relaxation protocol: the Hamiltonian size is reduced by diagonalizing within specific, symmetry-matched sub-blocks.

This group relaxation yields highly refined adiabatic aggregate states that minimize total energy while completely retaining their diabatic interpretability. By providing a scalable, atomistic resolution of complex electronic couplings, this tensor-product framework not only captures the gateway biexciton mechanisms previously identified but establishes a predictive foundation for designing robust multiexcitonic materials for next-generation light-harvesting and quantum technologies.

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LONG- AND SHORT-RANGE ELECTRONIC COUPLING IN PARA VS. META CONJUGATION ON SINGLET FISSION

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Solar cells represent one of the most promising solutions to address the growing global energy demand. However, the power conversion efficiency of single-junction architectures is fundamentally limited to around 33% due to various loss mechanisms. One significant source of loss is thermalization, where the excess energy of high-energy photons is dissipated as heat.[1] Strategies such as multiple exciton generation (MEG) and its molecular analogue, singlet fission (SF), offer pathways to surpass this efficiency limit by generating multiple charge carriers from a single high-energy photon.[2]

Singlet fission is a spin-allowed down-conversion process in which the excitation of a single chromophore leads to the formation of a correlated triplet pair. These triplet pair states may subsequently decorrelate into two independent triplets, potentially doubling the number of excitons produced.[3] Linear acenes, particularly pentacene dimers, have emerged as prototypical platforms for investigating SF. A critical design parameter in optimizing the SF efficiency is the linker connecting the pentacene units: It must facilitate both a high triplet pair quantum yield as well as efficient separation of these triplet pairs.[4]

In this study, we examine how extending the conjugated linker affects *intra*molecular SF (*i*-SF). Specifically, we focus on a series of *meta*- and *para*-connected pentacene dimers, which previously exhibited high triplet pair quantum yields but limited triplet separation due to strong inter-chromophore coupling.[5] By incorporating phenylacetylene units of varying lengths as linkers, we modulate this coupling and probe its influence on the SF dynamics. A combination of steady state and transient absorption (TA) spectroscopy is employed to systematically investigate how linker length impacts the efficiency and kinetics of *i*-SF.

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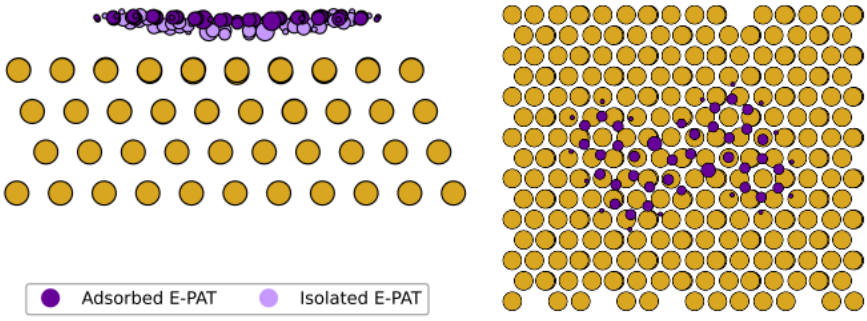
POSTERS

ADSORPTION-INDUCED STRUCTURAL AND OPTICAL CHANGES OF A THIOINDIGO-TYPE PHOTOSWITCH ON AU(111)

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Peri-anthracenethioindigo (PAT) is an all-red-light-responsive indigoid photoswitch whose extended π-conjugation enables switching in the visible and near-infrared spectral region [1]. A distinctive feature of PAT is the pronounced structural difference between its bowl-shaped *E*-isomer and step-like *Z*-isomer in solution [1,2]. Isomerization therefore requires substantial geometric flattening of the molecule and was previously found to proceed exclusively on the triplet manifold [2]. These unique structural and photophysical properties make PAT a promising building block for dye-sensitized functional materials and optically responsive surfaces. However, practical applications require immobilization on surfaces, where molecule-surface interactions may significantly alter both the geometric and electronic structure of the molecule, raising the question whether the characteristic switching behavior of PAT can be retained upon adsorption on metallic substrates.

Here, we employ density functional theory (DFT) and time-dependent DFT to investigate the structural and optical properties of PAT adsorbed on Au(111). We analyze the adsorption of the *E*- and *Z*-isomers as well as twisted intermediate structures relevant to the switching pathway. Our calculations reveal pronounced surface-induced flattening of the molecule, substantially reducing the geometric differences between the two isomeric forms. Exciton analyses further shows how adsorption modifies the nature and energetic position of the low-energy optical excitations. Overall, the results provide insights at the molecular level suggesting that PAT is likely to be capable of switching more efficiently and rapidly due to the molecule becoming flattened following adsorption onto the gold surface, yet still retaining the ability to be excited by all-red light.



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HAMILTONIAN LEARNING WITH GW-ACCURACY IN SOLIDS

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Accurate prediction of optoelectronic properties under realistic conditions is essential for understanding and designing next-generation semiconductor materials. However, treating large, thermally disordered systems with high-level electronic-structure methods remains computationally prohibitive. Recently, HAMSTER was introduced as a physics-informed Hamiltonian-learning framework that combines an approximate tight-binding description with machine-learned corrections to capture dynamic environmental effects in complex materials [1]. This enables interpretable and scalable predictions of electronic properties for systems far beyond the size accessible to direct first-principles calculations.

In this work, we present an ongoing extension of HAMSTER aimed at Hamiltonian learning with more accurate electronic structure. The central goal is to incorporate quasiparticle effects from many-body perturbation theory, in particular the GW approximation [2], into the HAMSTER workflow. While conventional, local density functional theory provides an efficient reference for training, it often underestimates band gaps and can misrepresent band-edge energetics. GW calculations improve the description of quasiparticle energies, but their computational cost limits their direct use for finite-temperature trajectories, disordered supercells, and large-scale simulations.

Our strategy is to use a small number of representative GW calculations to learn corrections to the effective Hamiltonian in the compact HAMSTER basis. By combining these higher-level electronic-structure targets with the existing physics-informed learning approach, we aim to transfer GW-level accuracy from small reference systems to large atomistic structures sampled from molecular dynamics. Initial applications will focus on halide perovskites, where thermal disorder and anharmonic lattice dynamics make accurate band-edge and band-gap predictions particularly challenging. This development opens a route toward GW-informed optoelectronic property predictions for realistic materials systems, while retaining the efficiency, interpretability, and scalability of HAMSTER.

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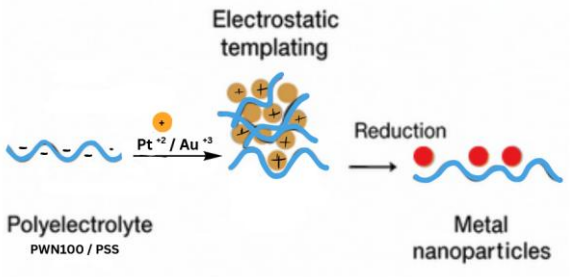
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POLYELECTROLYTE-DIRECTED PLATINUM NANOSTRUCTURES FOR CATALYTIC APPLICATIONS

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This project investigates the formation, structure and catalytic behavior of platinum nanostructures within two polyelectrolyte systems: a custom-designed phosphonated fluorinated polystyrene and commercial poly(styrene sulfonate) (PSS). The goal is to design novel systems for photocatalysis. We use “electrostatic nanotemplating to create particles in aqueous solution: Dicationic tetraammineplatinum(II) ions accumulate inside the oppositely charged polyelectrolyte and controlled reduction using sodium borohydride ($NaBH_4$) was employed to synthesize platinum nanoparticles within the polymer matrix. For exploiting their function, it is important to understand how platinum ions (Pt^{2+}) interact with negatively charged polymer chains in aqueous solutions. By varying the polymer concentration and the Pt^{2+}/polymer charge ratio, we monitored changes in hydrodynamic radius using dynamic light scattering (DLS) and evaluated the extent of metal ion binding and subsequent reduction. Results reveal that both polyelectrolytes exhibit distinct binding and aggregation behaviors due to their differing charge densities and backbone structures. Post-reduction analysis confirmed nanoparticle formation, with optimal stability observed at intermediate charge ratios. These particles are currently tested as novel catalyst systems. This study provides insights into the templating role of polyelectrolytes in nanomaterial synthesis systems for various possible future catalytic or functions and applications.



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HELICALLY CHIRAL ORGANOBORON COMPOUNDS: AZABOROLE- AND DIAZABOREPIN-TYPE-FUSED HELICAL SYSTEMS

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Helicenes are *ortho*-fused polycyclic aromatic hydrocarbons with extended π-conjugation and a helical, non-planar geometry that imparts inherent chirality. Incorporation of a trivalent boron atom is an effective strategy to tune the electronic and optical properties of helicenes perturbing their frontier molecular orbitals [1,2]. On the other hand, the Lewis acidic nature of boron makes them sensitive to air and moisture. Introducing an adjacent nitrogen donor mitigates this through intramolecular N→B coordination, thus enhancing stability of the system. We aim to integrate the unique properties of boron and the inherent chirality of helicenes to synthesize functional materials exhibiting distinct optical properties and enhanced performance compared to purely carbon-based analogs. We further seek to incorporate seven-membered diazaborepin (DAB) rings into the helicene framework, thereby extending BN-ring size and replacing the C^N-chelating motif with an N^N-chelating framework as design parameters for tuning the structural, chiroptical and electronic properties of BN-doped helicenes [3]. Herein, we present the synthesis, spectroscopy and comprehensive computational investigation of the fused helical systems containing 2*H*-1,2-azaborole and a diazaborepin-type motif, and systematically compare their structural, photophysical, and chiroptical properties to establish the impact of ring-size expansion and heteroatom doping.

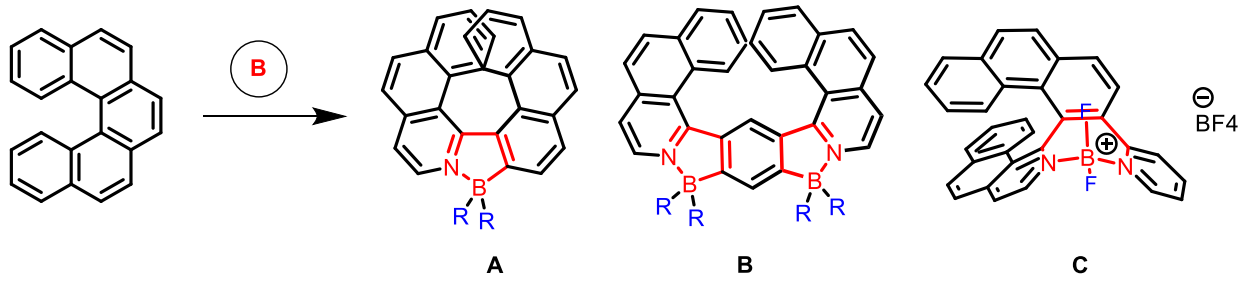


Figure 1. Examples of boron-nitrogen (BN)-doped helicene derivatives: (**A**) mono-BN-embedded helicene; (**B**) expanded bis-BN-doped helical framework; and (**C**) a cationic helicene incorporating a diazaborepin ring.

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TOWARDS SELF-CONSISTENT HUBBARD-CORRECTED DENSITY FUNCTIONAL THEORY

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Density Functional Theory (DFT) has long been the tool of choice for the study of the properties of molecule clusters and periodic solids. The main approximation of DFT is given by the expression of the so called exchange-correlation energy functional of the electronic density.

One popular way of dealing with this issue is a fractional inclusion of the Hartree-Fock energy within the total energy function of DFT (*Hybrid functionals*). Practically, this significantly increases the overall accuracy for material property predictions. However, it also comes at the cost of often empirical parameter choices and a high computational cost of the overall method compared to pure local or semi-local exchange-correlation functionals [1].

The Hubbard model consists of a model Hamiltonian that can, despite its simplicity, qualitatively correctly describe Mott insulators. Inspired by this Hamiltonian, one can add a Hubbard-like electronic energy correction to the DFT energy functional. For one of the parameters that arise in this model, usually referred to as U in literature, approaches for self consistent determination within a single DFT calculation exist [2]. Other parameters, determining so called Hubbard projectors, are still usually selected upon availability of different functions for different DFT code frameworks. This of course leaves ambiguity of the method itself, making projector choices empirical [3].

This work investigates properties of Hubbard projectors and their influence on electronic structure. We were able to show that using an appropriate parameter space the bandgap of model systems can be tuned within a significant value range, which emphasizes the importance of the choice of projectors, that is in turn mostly ignored or underestimated in current publications using DFT+U as a tool.

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IMPROVING PHOTOELECTROCHEMICAL NITRATE REDUCTION ON COPPER OXIDE ELECTRODES

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The photoelectrochemical (PEC) nitrate reduction reaction (NO_3RR) offers a green approach to simultaneous ambient ammonia (NH_3) production and nitrate (NO_3^-) removal from wastewater. Recent studies have shown this method is feasible using a cuprous oxide (Cu_2O) semiconductor as the catalyst [1], which is already recognized for its high NH_3 selectivity in electrochemical (EC) NO_3RR [2]. While the PEC approach was successfully demonstrated in a neutral electrolyte, the catalyst and reaction conditions require further optimization, particularly to match the high NH_3 selectivity of the EC reaction.

We compare the PEC-NO_3RR performance of Cu_2O, cupric oxide (CuO), and Kusachiite ($CuBi_2O_4$) (Figure 1). Cu_2O shows the highest nitrite (NO_2^-) yield and Faradaic efficiency, owing to its balance between activity and stability. However, neither material generates NH_3 under the initial conditions (0.3 V vs RHE, pH 13), necessitating further exploration. We find that the PEC-NO_3RR performance of Cu_2O in alkaline aqueous electrolyte exceeds that in neutral electrolyte. While the primary reaction product remains NO_2^- from 0.6 to 0.0 V vs RHE, NH_3 selectivity increases at lower potentials. However, under illumination at potentials < 0.3 V vs. RHE, Cu_2O is rapidly reduced to metallic Cu, promoting EC- rather than PEC-NO_3RR. We therefore explore possible strategies to reduce in-situ decomposition of the Cu_2O photoabsorber. Our results indicate that direct illumination could lead to significant efficiency gains in NO_3RR (photo)electrocatalysis, helping this technology move closer to commercial application.

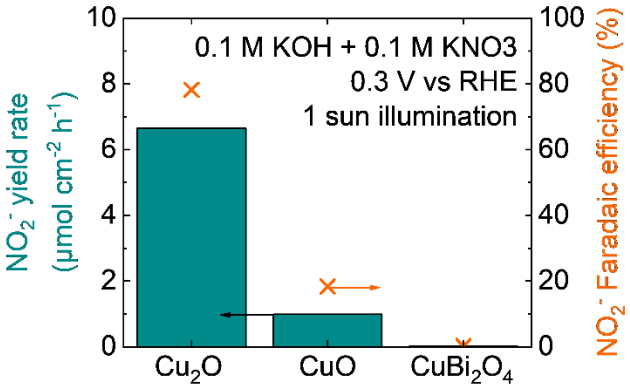


Figure 1. NO_2^- yield rate and Faradaic efficiency by material measured after 1 h photoelectrochemical NO_3^- reduction experiments on copper oxide-based photoelectrodes.

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STABILITY AND UNIFORMITY ENGINEERING IN PEROVSKITE NANOPARTICLES FOR ENHANCED PERFORMANCE

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Lead halide perovskite nanoparticles possess exceptional optical and electronic properties, yet their practical implementation remains limited by instability and non-uniformity at the nanoscale. In this work, we present a set of simple and scalable room-temperature strategies—based on compositional tuning, doping, and polymer-assisted synthesis—to engineer perovskite nanoparticles with improved stability, size uniformity, and enhanced luminescence. These approaches strengthen surface passivation, mitigate degradation pathways, and enable better control over the structural features that govern optical and electronic behavior. Across multiple perovskite compositions, the developed methods yield nanoparticles with higher quantum yields, improved photophysical responses, and more uniform emissive characteristics. In addition, selected materials were successfully integrated as down-shifting layers on silicon-based devices, demonstrating that nanoscale engineering directly translates into enhanced light-management performance at the device level. By advancing practical and accessible routes for producing robust perovskite nanoparticles, this work contributes to a deeper understanding of how nanoscale structure and chemical environment influence optical and electronic properties. These insights are relevant for applications ranging from light emission to energy conversion, and complement ongoing efforts to unravel charge transport and light–matter interactions on ultrashort length and time scales[1], [2], [3].

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QUANTIFYING THERMAL, PHOTOVOLTAGE, AND DEFECT CONTRIBUTIONS TO TRANSIENT ABSORPTION OF Ta_3N_5 PHOTOANODES

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Understanding how photogenerated charges relax in semiconductor photoelectrodes is essential for improving solar fuel devices, but transient optical signals often contain overlapping contributions that are difficult to assign unambiguously. This challenge is particularly relevant for Ta_3N_5, a widely investigated photoanode material for solar-driven water splitting whose performance remains strongly affected by short carrier lifetimes and defect-mediated recombination. In this work, microsecond-to-second transient absorption spectroscopy of Ta_3N_5 thin films is combined with complementary optical measurements to separate spectral signatures associated with lattice heating, electrostatic perturbations, and defect states. Photoreflectance spectroscopy resolves three critical points in the Ta_3N_5 band structure: two anisotropic near-band-edge transitions at 2.14 and 2.27 eV, and a higher-energy transition near 2.80 eV. These transitions closely match the dominant features observed in transient absorption spectra. The analysis reveals that a previously unreported photoinduced absorption feature at 2.80 eV originates from pump-induced lattice heating, while potential-dependent measurements show that the near-edge bleach signals are governed by pump-induced band flattening and subsequent surface photovoltage relaxation. By fitting the transient spectra using independently determined thermal and electrostatic components, the temporal evolution of both heating and photovoltage can be quantified. In parallel, the sub-bandgap response tracks changes in defect charge-state populations. These results provide a quantitative basis for separating thermal, electrostatic, and defect-mediated contributions to transient absorption spectra, offering a broadly applicable route to interpreting photoexcitation and relaxation processes in semiconductor photoelectrodes.

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IMPACTING THE BALANCE BETWEEN CO_2 AND PROTON REDUCTION BY CONTROL OVER AGGREGATION IN A MODEL π-CONJUGATED N-HETEROCYCLE – PROFLAVINE

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We investigated the mechanistic factors that govern the selective photocatalytic reduction of CO_2 over protons within a simple π-conjugated N-heterocycle, proflavine. (Figure 1) Diluted conditions, where aggregates of 65 nm are formed, favored the selective CO_2 photo-reduction, while the gradual transition to concentrated conditions enabled photo-reductive H_2 generation. Proton reduction is coupled to larger aggregates, in which an alternative photo-relaxation pathway is active. We used transient absorption spectroscopy to corroborate, that at low proflavine concentrations the presence of an electron donor triggers the one-electron reduced proflavine to perform the direct CO_2 reduction. At high proflavine concentrations, protonation of the one-electron reduced proflavine was favored due to a positive shift in basicity in larger aggregates with sizes over 1 µm. In turn, H_2 abstraction began with a pair of one-electron reduced, protonated, intermediates. Our study demonstrates an effective approach to limiting water reduction, a key challenge in advanced metal-free organic photocatalysis.

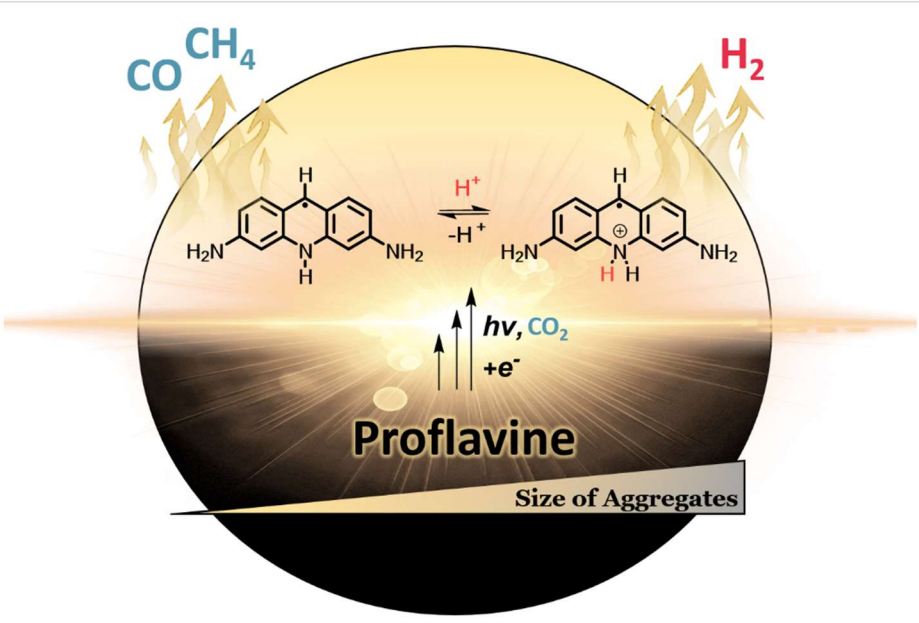


Figure 1: Reaction scheme of proflavine highlighting the influence of aggregation on its photocatalytic behavior.

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INVESTIGATION OF SYMMETRY BREAKING CHARGE TRANSFER IN PHTHALOCYANINE DIMERS

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Photoinduced symmetry breaking charge transfer (SB-CT) has garnered considerable attention in the scientific community owing to its pivotal role in maximizing energy conversion efficiency in artificial light-harvesting systems. It is an excited state process where a symmetrical pair of identical chromophore leads to the formation of an asymmetric charge separated state upon photon absorption [1]. In comparison with the traditional electron donor-acceptor systems, SB-CT facilitates the charge separation with minimal energy loss [2]. Multichromophoric systems that exhibiting SB-CT mimic the light capturing and charge separation process in natural light harvesting systems, with the potential to outperform conventional electron donor-acceptor systems. In this study, excited state dynamics in a series of phthalocyanine dimers are investigated by means of steady-state absorption and fluorescence spectroscopy, transient absorption spectroscopy, and electrochemical methods. In general, the rate of SB-CT process depends heavily on the electronic coupling strength between the phthalocyanines and the solvent environment [3]. Consequently, we also examined the influence of aforementioned factors on the photodynamics of phthalocyanine dimers.

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QUANTIFYING ELECTRON TRANSFER FLOWS WITH REAL-TIME DENSITY FUNCTIONAL THEORY

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Tungsten Trioxide (WO_3) is attractive as a photoanode for photoelectrochemical water splitting. In a joint experimental and theoretical effort [1] we investigate the rate limiting step in photoelectrochemical water splitting, which is the oxidation of water. To enhance the accessible surface area and thus the overall performance, mesoporous photoanodes composed of WO_3 nanoparticles are going to be realized. Additionally, we attempt to further increase the efficiency of the reaction by catalyzing it with active complexes that are anchored to the WO_3 surface [2].

For such complexes to effectively drive the oxidation reaction, efficient electron transfer from the anchoring ligand to the WO_3 cluster or surface slab is essential: Upon photoexcitation, electron holes are generated in the semiconductor. Once stabilized they can be utilized for water oxidation. In this process, the ligand acts as an electron acceptor, initiating the reaction by transferring electrons from the water molecules to the WO_3 as part of the oxidation step. The efficiency of this process critically depends on the strength and dynamics of the electron flow between the ligand and the WO_3 system.

This work focuses on quantifying the extent of electron transfer – specifically, electron flow from the ligand to a WO_3 cluster or surface slab – using real-time density functional theory. To this end, three distinct computational approaches were developed to model and analyze electron transfer between the ligand and the WO_3 system. Furthermore, we present a calculation to derive a measure of electrical conductivity, offering additional insight into the electron transfer properties.

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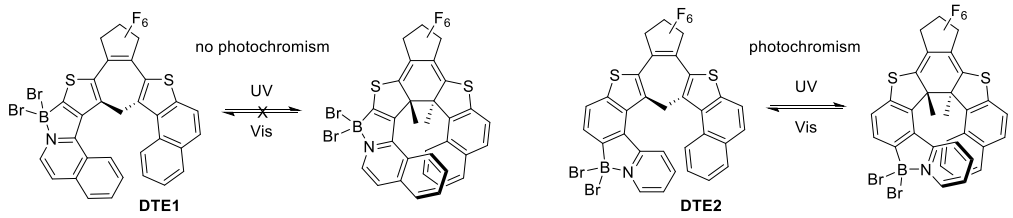
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AZABOROLE-CONTAINING DIARYLETHENE PHOTOSWITCHES

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The incorporation of boron into polycyclic aromatic hydrocarbons (PAHs) has emerged as a versatile strategy for tuning the electronic and optical properties of π-conjugated systems [1]. Extending this concept to photoresponsive materials is particularly attractive, as boron incorporation offers new opportunities to modulate the photophysical behavior of molecular switches. Among the various classes of photoswitches, diarylethenes (DAEs) are particularly attractive due to their high thermal stability, fatigue resistance, and reversible light-induced ring-closing and ring-opening reactions [2]. Previous studies have demonstrated that azaborole units can be incorporated into helically extended π-conjugated frameworks.[3] However, the integration of an azaborole and the photoactive DAE framework into the helical structure remains unexplored.



Scheme 1. Structure-dependent photochromism of azaborole-containing diarylethenes **DTE1** and **DTE2**.

The poster presents the synthesis and photophysical characterization of two DAE photoswitches in which boron is incorporated into the helical scaffold. **DTE1** and **DTE2** (Scheme 1) differ only in the position of the azaborole unit. Interestingly, **DTE1** exhibited no detectable photochromic activity, whereas **DTE2** readily underwent reversible photocyclization accompanied by a distinct color change from yellow to red.

To explain the contrasting behavior of both photoswitches, theoretical calculations and transient absorption spectroscopy were employed. The resulting mechanistic insights into the excited-state processes enabling the 6π-electrocyclization and the origin of the observed structure-dependent photochromism will be presented.

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PTHS: A POLYELECTROLYTE P3HT-DERIVATIVE FOR SEQUENTIALLY PROCESSED BILAYER OSCS

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Poly(3-hexylthiophene) (P3HT) is a well-researched donor polymer for application in organic solar cells (OSCs). Side chain modification of P3HT with sulfonate groups yields Poly(6-(thiophene-3-yl)hexane-1-sulfonate) (PTHS), a polyelectrolytic donor polymer with high hole transport mobility [1]. This polyelectrolyte possesses two key advantages:

Firstly, exchange of the cationic counter ions enables insolubilization of the donor layer, allowing simple fabrication of donor-acceptor bilayer systems by sequential spin coating (Figure 1). This simple process enables the construction of bilayer solar cells with a wide variety of acceptors, including both fullerene and non-fullerene acceptors (NFAs).

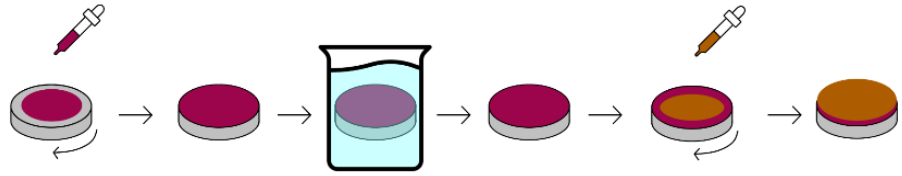


Figure 1: Schematic of the ion exchange and sequential spin coating process.

Secondly, adjusting the counter ion composition enables tuning of the donor energy level, which is critical for achieving high open circuit voltages (V_{OC}) [2].

X-ray photoelectron spectroscopy (XPS) measurements confirm successful cation exchange with K^+, Na^+, Li^+ and Ca^{2+} by dipping PTHS films into saturated aqueous solutions of the respective chloride salts. Using the sequential spin coating process, bilayer solar cells are produced with PCBM as a fullerene acceptor and compared to NFA devices. By utilizing different cations, the donor-acceptor energy level offset (E_{off}) can be varied and its effect on charge generation efficiency can be studied in these devices. This allows for investigations into the role of E_{off} as a critical driving force for charge generation in organic solar cells [3]. Bilayer devices are well suited for this purpose, because they avoid the uncertainty in interfacial energy levels and interfacial area that is inherent in bulk heterojunction devices [4].

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TOWARDS CD-SPECTROSCOPY OF SINGLE CHLOROSOMES

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As one of the most efficient light-harvesting systems in nature chlorosomes (the light-harvesting aggregates of green-(non)-sulfur bacteria) are considered as a template for novel solar cells [1]. Among other techniques linear-polarization resolved fluorescence-excitation spectroscopy revealed molecular aggregates of cylindrical symmetry as the dominating secondary structural elements within the chlorosomes [2]. Development of circular-dichroism spectroscopy will allow to elucidate further structural details such as the diameter and the length of the cylindrical structures.

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HOW TO FIX SILVER FOR PLASMONICS?

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Silver (Ag) is an ideal metal for plasmonic applications in the visible regime, but its use is hindered by the low chemical stability and poor structural quality of thermally evaporated thin films and nanostructures. Here, we present a simple approach to overcome these limitations by alloying Ag thin films with small amounts of gold (Au) through thermal co-evaporation. We analyzed $Ag_{100-x}Au_x$ thin films with Au contents ranging from 5 to 20 at.% with respect to their surface and bulk crystal quality, optical properties and chemical stability. Our results show that low Au concentrations significantly reduce the surface roughness of co-evaporated thin films and significantly enhance their chemical stability, while maintaining a defined crystalline growth (Figure 1). These improvements are achieved without metallic wetting layers, epitaxial substrates or template stripping. Among the compositions studied, $Ag_{95}Au_5$ thin films exhibit the highest chemical stability, lowest optical losses in the visible spectral range, and excellent plasmonic properties even outcompeting those of pure Ag.
As proof of concept, we fabricate $Ag_{95}Au_5$ plasmonic nanoantennas of different geometries and resonances (Figure 1) demonstrating excellent long-term durability over one month under ambient conditions. Our approach thus demonstrates a practical solution to combine the superior optical properties of Ag with the chemical stability of Au for future plasmonic applications [1].

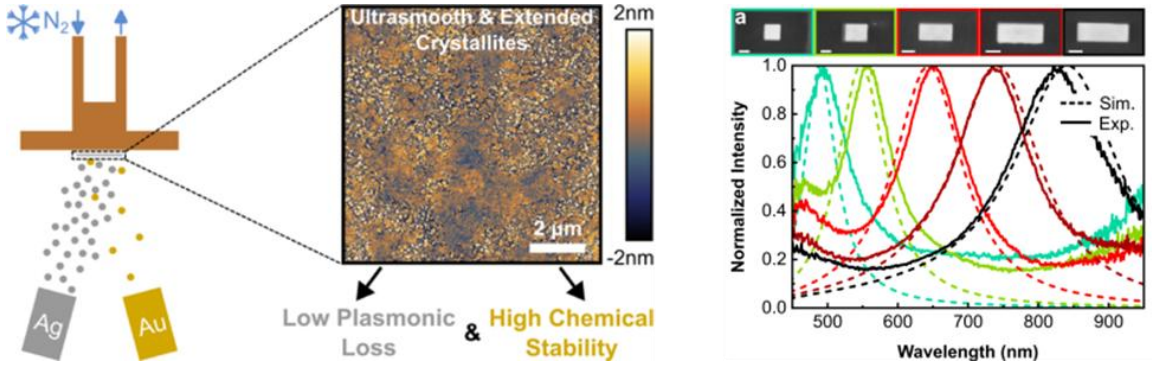


Figure 1: By alloying silver (Ag) with small amounts of gold (Au) through thermal co-evaporation, we are able to fabricate ultrasmooth, chemically stable thin films with excellent plasmonic properties. As proof of concept, we fabricate $Ag_{95}Au_5$ plasmonic nanoantennas. [1]

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PHASE SEGREGATION IN MIXED HALIDE PEROVSKITES: RECONCILING MECHANISTIC AND THERMODYNAMIC MODELS

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Mixed halide perovskites have emerged as leading contenders for multi-junction solar cells due to their tunable band gaps, controlled by halide composition, and excellent optoelectronic properties. However, compounds such as $MAPbI_{3-x}Br_x$, suffer from light-induced halide segregation, resulting in compositional heterogeneity that degrades device performance.

Despite extensive experimental and theoretical efforts, the physical origin of light-induced halide segregation in mixed-halide perovskites remains debated. Several driving forces have been proposed, including polaronic strain [1], band-gap-driven carrier stabilization [2], internal electric fields [3], and photo-induced redox processes [4]. While each model captures specific aspects of the phenomenon, seemingly similar experimental observations are often interpreted differently across the literature.

We compare the underlying assumptions, predictions, and experimental signatures of these models and argue that many apparent inconsistencies arise from insufficient separation of kinetic and thermodynamic aspects. Specifically, the segregation rate is largely governed by halide migration kinetics, whereas the final extent of segregation is determined by the underlying free-energy landscape. [5]

We propose that the latter can be described within a generalized thermodynamic framework, in which different microscopic models correspond to different ways of modifying the free-energy balance under illumination. The separation of kinetic and thermodynamic aspects provides a basis for more comparable experimental studies. Building on this, we employ targeted investigations on mixed cation systems and tailored additives to distinguish between contemporary models and elucidate the physical origins of halide segregation.

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EXPLORING HETEROJUNCTIONS OF BI-FUNCTIONAL MATERIALS FOR NEW SOLAR BATTERY DESIGNS

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Driven by climate change, there is growing interest to increase the utilization and efficiency of renewable energy, particularly solar cells to leverage the abundance of solar energy. The intermittency of solar energy further motivates research into new energy storage solutions. Therefore, solar batteries (SBs) which integrate light-harvesting and electrochemical charge storage into one device are gaining renewed interest, after being first developed by Hodes in 1976 [1]. Bi-functional materials which are both photoactive and charge-storing, such as potassium poly(heptazine) imide (K-PHI) [2], show strong promise as photoanode candidates for solar batteries [3].
In this work we investigate K-PHI as a photoanode across multiple solar battery designs as depicted in Figure 1. Spectroscopic and photoelectrochemical characterization of K-PHI/hole transport material (HTM) heterojunctions reveals the hole extraction capability of various HTMs. Furthermore, the performance of the photoanodes is tuned by optimizing film fabrication and developing a K-PHI-based composite.

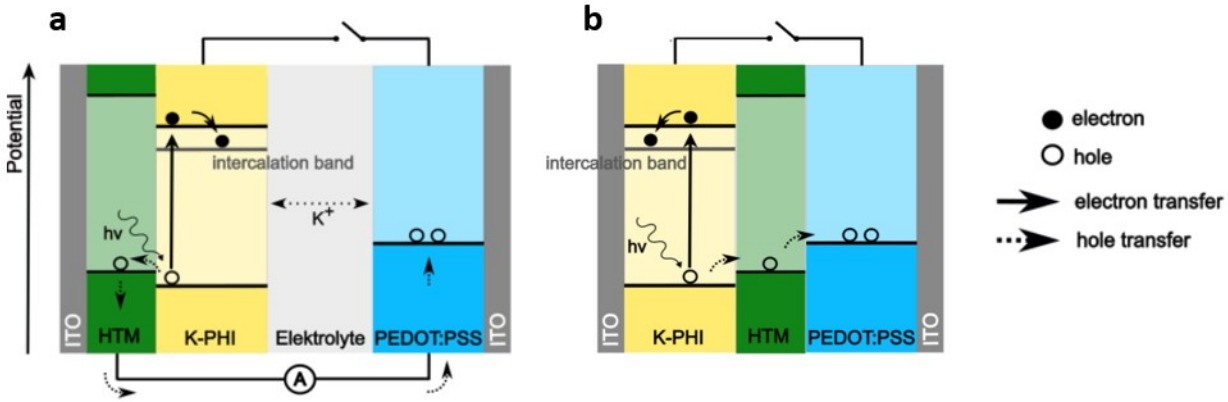


Figure 1: Schematic representation of the photocharging mechanism of photo-rechargeable SBs using K-PHI (yellow) as an electron-storing photoanode, PEDOT:PSS (blue) as the cathode and an HTM (green) to extract holes. The holes are transported to the cathode (a) externally via wires or (b) internally via the HTM.

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PLASMON-ASSISTED LITHIUM-IONS CAPTURE

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The growing demand for lithium has recently prompted the exploration of advanced materials with tailored ion selectivity and enhanced reaction kinetic to further lower the price of lithium recovery. Industrially, lithium is mainly obtained through the utilization of evaporation ponds, but unfortunately, this is a highly time-consuming process, polluting, it relies on atmospheric conditions, and is thus expensive [1].

In this work we prepared core-shells nanoparticles combining gold cores and shells made of materials able to selectively capture lithium-ions (lithium aluminium layered double hydroxides [LiAl-LDHs], and manganese oxide). In these structures the core acts as a photo-heater to adsorb visible light and then locally increase the temperature of the shell that is responsible for the Li capture.

The nanoparticles were colloidally synthesized, and then characterized. Lithium capture under dark and under illumination was then evaluated, also in simulated salt brines. Following particle synthesis, the core–shell structures were incorporated into composite membrane systems to explore their potential implementation in realistic membrane-based applications.

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Translation of Covalent Organic Framework Catalysts from H-Cell to Flow Cell Conditions for CO_2 Electroreduction

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The current climate crisis can be addressed by lowering CO_2 levels and transforming CO_2 into chemical energy and value-added chemicals. Electrochemical CO_2 reduction reaction (eCO_2RR) could contribute to storing renewable energy, once available on an industrial scale. Covalent organic frameworks (COFs) are reticular materials distinguished by high tunability, porosity, and well-defined structures. These properties render COFs as potent catalysts for eCO_2RR.[1] However, most reported studies rely on non-scalable H-cell configurations, limiting insights into performance under harsher industrially relevant conditions, which can compromise COF stability and catalytic performance. In this work, we investigate benchmark COF-366-Co as a catalyst layer for gas diffusion electrodes in a membrane electrode assembly electrolyzer. We examine the influence of ink formulation and electrode fabrication methods on the structural integrity and electrochemical performance of COFs. (Figure 1).[1,2] Additionally, we evaluate the effect of chemical linkage on the performance by post-synthetic reduction into amine-linked (AR-COF-366-Co) and by direct synthesis of a new analogue COF with a benzothiazole-linked backbone (TZ-COF-366-Co) for eCO_2RR in flow cell architectures. We evaluate the activity and stability of the catalysts by post-mortem characterization to assess structural degradation and performance correlations based on the structural changes. Our findings underscore the critical need to align COF synthesis and electrode fabrication strategies with operational conditions to unlock their full potential in scalable eCO_2RR technologies.

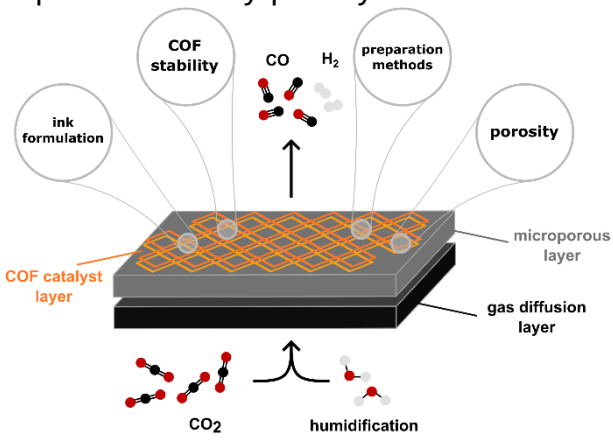


Figure 1. Schematic representation of relevant aspects of gas diffusion electrode preparation with COFs for eCO_2RR.

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PORPHYRIN-FUSED HELICAL MULTILAYER NANOGRAPHENES

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Helical nanographenes have gained considerable attention due to their non-planar π-conjugated structures and chiroptical properties. Increasing the size of the π-system and introducing multilayer arrangements can significantly affect their electronic and photophysical properties [1,2].

In this work, porphyrins are incorporated into helical multilayer nanographene systems. Ethynyl-functionalized phenanthrene building blocks are used to form extended aromatic structures by Diels–Alder reactions and oxidative cyclodehydrogenation. Oxidative *β-meso* five-membered ring fusion is subsequently used to connect the porphyrin units directly to the nanographene π-system [3,4].

The synthesized compounds will be characterized to study the influence of porphyrin fusion on the structural, optical and electronic properties of the helical π-systems.

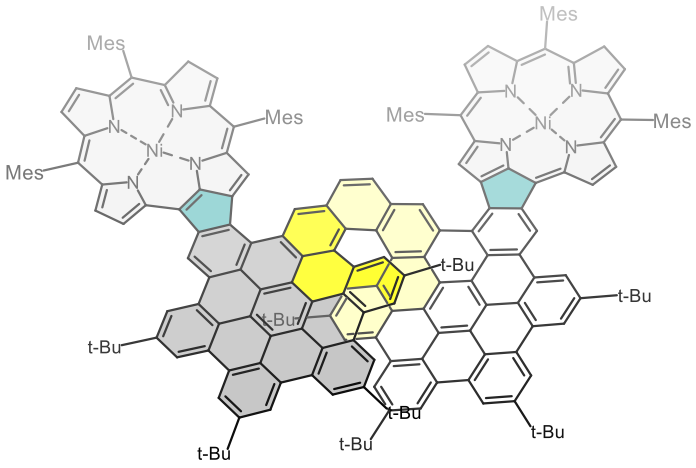


Figure 1. example of π-extended porphyrin-containing helical nanographene system.

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CHIRAL N-ATOM DOPED NANOGRAPHENES

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Chiral nanographenes combine the unique properties of inherently chiral molecules with the optical, electronic and magnetic properties of nanographenes. [1] This fascinating class of polycyclic aromatic hydrocarbon structures can find new applications in the field of nanoelectronics, optoelectronics and spintronics. [2]

Another strategy to modulate the properties of graphene is doping with heteroatoms, which can induce exotic features such as ferromagnetism but most importantly it can enhance the conductivity of the material and promote the formation of a band gap. [3,4]

By combining chirality and doping, a new set of optoelectronic and photophysical properties can be generated, opening a new field of potential applications in nanoelectronics. [2,3]

In this work, so called pyridinic nanographenes are linked with the inherently chiral molecule spirobifluorene by different cross-coupling reactions and subsequent Scholl oxidation.

The synthesized compounds will be characterized to study the influence of contortion and doping on the structural, optical and electronic properties of presented systems.

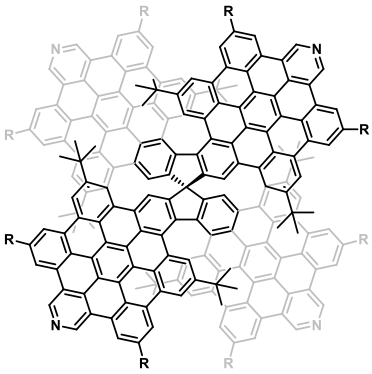


Figure 1: Example of Chiral Pyridinic Nanographene.

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ADVANCED SPECTROSCOPY AND EMISSION LINESHAPES: UNCOVERING EXCITONIC BEHAVIOR IN PEROVSKITES

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Analysis of photoluminescence (PL) spectra is a ubiquitous and essential tool in semiconductor research. Ensemble PL spectra are commonly evaluated using Voigt profiles; however, their microscopic origin often remains unclear. In perovskite nanocrystals, quantum confinement and exciton–phonon interactions play a significant role in shaping the PL emission profile. The Gaussian-asymmetric Laplace (GaLa) fitting algorithm developed by our group correlates characteristic PL lineshape features with nanocrystal ensemble statistics [1].

Temperature-dependent PL measurements from cryogenic to room temperature provide a particularly insightful test case. Using the GaLa approach, the thermal broadening encoded in the Boltzmann-distributed high-energy wing of the PL spectrum can be reproduced with remarkable accuracy.

Optimizing optical lineshapes for future optoelectronic devices is just as important as improving charge transport in thin films. Time-resolved PL (TR-PL) measurements enable advanced characterization of recombination dynamics, revealing decay pathways and dark–bright exciton splitting. Furthermore, TR-PL studies on homogeneous perovskite thin films allow quantification of exciton diffusion between nanocrystals via Förster resonance energy transfer (FRET) [2]. Exciton diffusion depends strongly on both ligand length and lateral nanocrystal size — parameters we are actively tuning and investigating.

Together, these spectroscopic approaches provide a comprehensive picture of excitonic behavior in perovskite nanomaterials, linking emission lineshapes, carrier dynamics, and nanoscale transport processes. By combining advanced spectral analysis with time-resolved techniques, we aim to establish design principles for perovskite systems with tailored optical and excitonic properties for next-generation optoelectronic applications.

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WHEN METALS BECOME MOLECULES

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When a metal is reduced to only a few atoms, it stops behaving like a metal. The continuous bands of the bulk give way to discrete, molecule-like electronic states, and the cluster acquires sharp, light-active properties that depend sensitively on its exact size and composition. These few-atom clusters are the smallest building blocks of the metal nanomaterials used in light-driven catalysis. How they absorb light, and where that energy goes, is of both fundamental and practical interest.

A reliable description of their electronic states is beyond conventional density functional theory. We turn instead to high-level multireference methods and, in synergy with experiment, resolve both the excited-state landscape and the nonradiative pathways by which absorbed energy is redistributed. Across gold, cerium, and silver clusters [1,2], this reveals excited-state behavior richer than their small size would suggest.

Together, these studies build a bottom-up picture in which the smallest clusters help explain the photophysics and catalysis of much larger metal nanomaterials.

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SINGLE-SITE WATER OXIDATION CATALYSIS WITHIN A HETEROGENOUS RUTHENIUM-CONTAINING ORGANIC FRAMEWORK

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Mimicking the oxygen evolving Photosystem II (OEC-PSII) has been a successful strategy for the design of supramolecular architectures for homogenous water oxidation catalysis.[1–3] The implementation of well-defined molecular water oxidation catalysts (WOCs) into framework materials would lead to heterogeneous catalysts with improved stability, recyclability and structural integrity. As one of the very few examples available in the literature so far, we recently reported on Ru(bda)-containing (bda = 2,2′-Bipyridine-6,6′-dicarboxylate) COF nanoparticles with excellent performance in heterogeneous water oxidation.[4] We expanded on this concept and report on the incorporation of Ru(bda) units as linear building blocks in COFs. The immobilization of Ru(bda) WOCs within the porous matrices significantly improved the stability of the catalysts and resulted in a heterogeneous WOC with excellent durability and performance.

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INVESTIGATION OF COVALENT DONOR-ACCEPTOR PBI FOLDAMERS EMPLOYING VARIOUS SPACER MOIETIES

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Solar energy harvesting via conversion of a photon into a charge separated state is fundamental to natural photosynthesis. To mimic natural photosynthesis, scientists gained in-depth knowledge investigating *π*-conjugated molecular donor-acceptor dyads and donor-bridge-acceptor triads.[1-2] A pronounced dependence of electron transfer (ET) rates on donor-acceptor-distance could be revealed, and their quality to achieve long-range ET has been described by an empirical attenuation factor *β*. However, these systems were limited to linear *π*-conjugated chains, resulting in a 'through-bond' ET.[3-4]

We recently reported on a series of highly defined, co-facially stacked donor-acceptor perylene bisimide (PBI) foldamers. Upon selective excitation of the donor, 'through stack' wire-like electron hopping was observed in polar solvents with a low attenuation factor of $\beta = 0.21$ Å^{-1}, being comparable to conjugated oligo-*p*-phenylene or -*p*-phenylene-ethylene bridges.[3-5] The co-facial arrangement of the PBI subunits results in substantial orbital overlap, yielding pronounced hole and electron transfer integrals, which are necessary for charge migration in stacks. These are highly sensitive to the orientation of the chromophores and should therefore be modulated by different connecting spacer units.[5] We hypothesize that an increased electron transfer integral will result in even faster charge transfer and smaller attenuation factors.

To test this hypothesis, a series of donor-acceptor dyads was prepared. Steady-state absorption and emission measurements were performed in solvents of varying polarity, as well as quantum chemical calculations to assess the electronic coupling of the chromophores. Time-resolved spectroscopy will be performed in the future to determine ET rates of charge separation and recombination.

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COMPOSITION TUNINING OF I-III-VI QUANTUM DOTS ENHANCES BAND-GAP EMISSION

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I-III-VI quantum dots (QDs) have been attracting significant attention in recent years due to their high stability and promising optical properties. [1] Further, their heavy-metal-free composition makes them environmentally friendly compared to their toxic counterparts: CdS, CdSe, and PbSe. While size-dependent tuning of optical properties due to quantum confinement is straightforward in QDs, composition-dependent control of emission and absorption in I-III-VI QDs is often challenging due to uncontrolled alloying and formation of defects. This leads to a broad and strongly red-shifted emission spectrum, limiting their use for light-emitting applications. Previously we have shown that shelling the core QDs with a higher band-gap material enhances recombination of excitons at the band-gap. [2] Here we focus on alloying and show, that this itself enhances band-gap emission in I-III-VI core QDs. By systematically varying the In to Ga ratio during synthesis, the band-gap and emission color of Ag-based I-III-VI QDs is tuned, resulting in quaternary $AgIn_xGa_{1-x}S_2$ QDs. Increasing Ga content in the system induces a blue shift in absorption and emission maxima due to band-gap widening. Hence, composition tuning enables us to achieve I-III-VI QDs covering the entire visible spectral range, making them highly versatile fluorophores.

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IN-SITU GISAXS STUDY OF FILM FORMATION IN LAYER-BY-LAYER PRINTED NON-FULLERENE ORGANIC SOLAR CELLS BASED ON GREEN SOLVENTS

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Layer-by-layer printing has emerged as a promising strategy for tailoring the morphology of non-fullerene organic solar cells (NF-OSCs). In contrast to conventional bulk heterojunction fabrication, which often leads to excessive phase separation and the formation of isolated donor- or acceptor-rich domains that hinder charge transport, [1] the layer-by-layer approach enables more controllable vertical phase distribution and interfacial organization, thereby offering potential improvements in device performance. [2]

In this work, the film formation process of layer-by-layer printed active layers is systematically investigated using in situ grazing-incidence wide-angle and small-angle X-ray scattering (GIWAXS/GISAXS). The system studied consists of the polymer donor PCE18 and the small-molecule acceptor BTP-4F, processed using a green solvent system to reduce environmental impact while maintaining film-forming quality and device-relevant morphology control.

The results reveal that during deposition, the donor material diffuses into the pre-formed acceptor layer, driving continuous structural evolution. Preliminary GIWAXS analysis shows a reduced π–π stacking distance and an increased crystalline coherence length (CCL) after donor deposition, indicating enhanced molecular ordering and more efficient charge-transport pathways. These findings demonstrate that layer-by-layer printing, particularly when combined with green solvent processing, can induce a highly ordered morphology favorable for photovoltaic performance in NF-OSCs.

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CONTROLLING THE FLOW OF CHARGES ACROSS PHTHALOCYANINE@TRANSITION-METAL DICHALCOGENIDE INTERFACES

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Exfoliated 2D transition metal dichalcogenide (TMDC) flakes provide a straightforward route to dispersed semiconductor samples, and they can also self-assemble at the liquid/liquid interface into semiconducting nanosheet networks (NNs) using the Langmuir –Schäfer technique. Their interaction with phthalocyanines (Pcs) opens up new functionalities for photocatalysis, photovoltaics and optoelectronics. Our studies focused on the energetic alignment of the Pc molecular orbitals with the TMDC bands, to understand how this alignment influences charge transfer (CT) across the interface.[1]–[3] The Pcs immobilized quasi-irreversibly on the TMDC surface in a face-on orientation, as confirmed by steady-state spectroscopy. In the absorption spectra, a new, shifted band appeared, while the Pc-centered fluorescence was quenched. This indicated electronic coupling between the constituents, which was further supported by theoretical calculations. Ground-state CT was characterized by X-ray photoelectron spectroscopy (XPS). Upon photoexcitation, these systems underwent interfacial charge separation, which was probed using transient absorption spectroscopy and showed the characteristic signatures of the Pc radical cation and/or radical anion, depending on the energetic alignment. These systems serve as a versatile platform for designing interfaces with specific properties, in particular charge transfer across the interface, by interchanging the metal center and/or the substituents of the phthalocyanines.

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LANGMUIR–BLODGETT ASSEMBLY OF PM6 AND N2200 POLYMER PLANAR HETEROJUNCTIONS FOR INTERFACIAL PROBING

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Precise control over thin-film interfacial organization is crucial for solution-processed organic electronics [1]. Here, we demonstrate the successful Langmuir–Blodgett (LB) fabrication of nanometer-precise, uniform PM6 and N2200 polymer films [2].

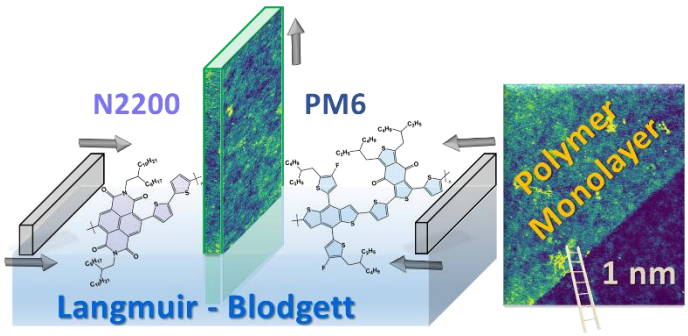


Figure 1. Langmuir-Blodgett assembly of high structural quality N2200 and PM6 polymer films in mono- and multilayer regimes providing direct access to the interfacial effects.

Optimized solvent and spreading conditions yield controlled assembly of uniform and homogeneous mono- and multilayers (Figure 1). PM6 formed isotropic films with tangled coiled structures, while N2200 showed anisotropic domains with directional π-stacking and extended branch-like polymer chains. Nanomechanical analysis revealed a 35–40% increase in surface elasticity for multilayers versus monolayers. Surface potential measurements underlined a thickness-dependent transition from substrate-dominated electrostatics in monolayers to a bulk-like behavior in multilayers, while photoluminescence mapping confirms preservation of emissive functionality even down to a monolayer. Preliminary photoresponsivity tests with photoactive layers below 20 nm show a reproducible increase in short-circuit current density upon increasing the number of PM6 and N2200 layers from five to six each, as confirmed by measurements across multiple devices. This trend is attributed to an absorption cross section that scales with increasing layer thickness. Our findings position the LB technique as a reliable approach for engineering ultrathin, structurally coherent, and electronically functional polymer interfaces with nanometer-scale thickness precision.

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PHOTOCATALYSIS WITH SELF-ASSEMBLED ORGANIC-INORGANIC HYBRID NANOSTRUCTURES

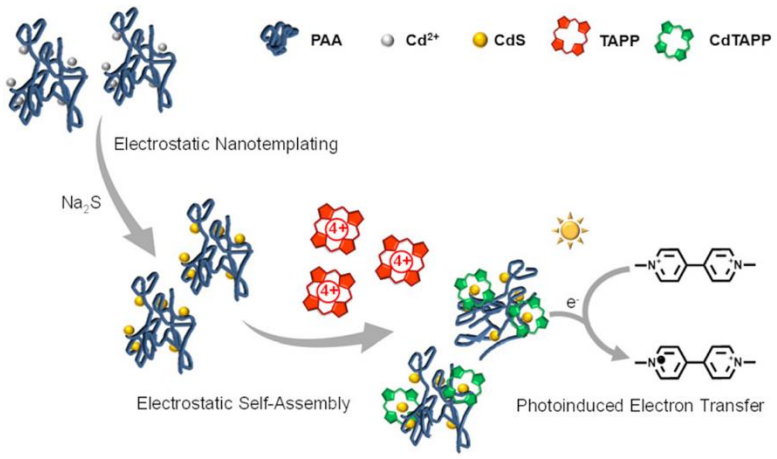
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Given the growing need for sustainable energy and processes and inspired by the photosynthesis of plants in Mother Nature, self-assembled photocatalysts are highly desirable, in particular in aqueous environments.

Spontaneous 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.

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 noble metal or semiconductor nanoparticles with a porphyrin as a light harvester, such that the photocatalytic activity is substantially enhanced. Key for a applications is to understand structure directing effects and structure-function relationships, while self-assembly offers a versatile and tunable principle for future target-desigend multi-component systems for solar energy conversion.



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PHOTOLUMINESCENT CORE-SUBSTITUTED NAPHTHALENE BISIMIDE HETEROCYCLOPHANE WITH PLANAR CHIRALITY

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Photoluminescent materials have been widely exploited for light-harvesting in areas of optoelectronics, bio-imaging, catalysis and sensing. Among these, host-guest complexes are advantageous, as the supramolecular interactions that enable complexation also assist in rigidification of the chromophoric moieties, thereby mitigating radiative deactivation pathways. Apart from conventional macrocyclic hosts such as cyclodextrins and cucurbiturils, macrocycles with emissive cores encapsulating chromophoric guests are particularly interesting, as they permit modulation of energy levels and photophysical properties, beyond rigidification effects. In this regard, arylene bisimide cyclophanes have been explored by our group as luminescent hosts, as they have π-surfaces facilitating high binding affinities hence expanding the choice of guest molecules.[1] Moreover, activation of accessible triplet excited states present in arylene bisimides to unlocking diverse excited state photophysics can be enabled by guest modulation.[2]

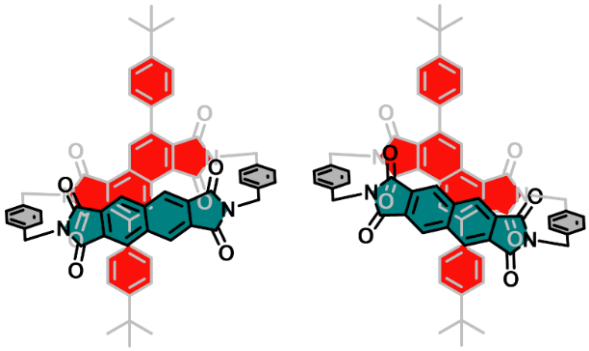


Figure 1. Enantiomeric pair of the core-substituted naphthalene bisimide heterocyclophane, NBI-HCy

Herein, a naphthalene bisimide based heterocyclophane, NBI-HCy, is presented as the host, where one of the naphthalene cores is substituted with *t*-butylphenyl groups (Figure 1). The design not only features increased π-surface area by core-substitution, but by employing two isomers of naphthalene bisimide as the cores, chirality is introduced, achieving circularly polarised luminescence (CPL).

The photophysical and chiroptical properties of the host are investigated and its ability to bind various guest molecules are experimented. NBI-HCy exhibits green CPL with an absorption dissymmetry factor of around 10^{-3} and a significant photoluminescence quantum yield of 45%. The binding constants reach as high as 10^{8} M^{-1} with electron-rich guests in carbontetrachloride forming charge transfer (CT) host-guest complexes, which is leveraged to obtain tunable CPL properties.

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COMPUTATIONAL DESIGN OF A FERROELECTRIC FRAMEWORK MATERIAL BASED ON DIPOLAR ROTORS

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Organic or metal-organic coordination framework materials are known for their versatility in terms of possible functions and properties. They can be synthesized to either be dense or yield wide open pores, they can be functionalized for sensing, storage, catalysis or transport of ions and—in some cases—also electrons. This versatility is mostly due to the wealth of potential molecular level modifications that the linking units can undergo. Very recently, it has been shown that it is even possible to synthesize linkers that incorporate rotatable dipolar groups, essentially making the framework material a dielectric. In all iterations to date, these rotors aligned randomly or antiferroelectric at practically relevant temperatures, yielding no net cell polarization, i.e. macroscopic ferroelectric poling. For various applications, like data storage, enhanced active and tuneable filters, nano rotators such that 3D lattice mounted crystalline rotors might be utilized as highly parallelized molecular machines, a ferroelectric framework material would be a great advantage, but could—to date—not be achieved. Part of this is due to the fact that, in contrast to inorganic ferroelectric materials, there is little to no theoretical guidance how a ferroelectric covalent or metal-organic coordination framework materials based on rotatable groups could be designed. For example, there is no analytically solvable equivalent to a 3D Ising or Potts model for general lattices with dipoles rotating around non-trivially aligned axes.

In this work, we present a hierarchical numeric approach to solve the design problem of 3-dimensionally aligned rotating groups. Using various levels of abstractions we uncover how different contributions to the total energy—ranging from the pure dipole, via more complex electrostatics, to non-electrostatic contributions such as van der Waals attraction and Pauli repulsion—influence the final alignment of the rotors. Finally, we present a prototypic framework that, according to simulations, should show a ferroelectric phase at finite temperatures.[1]

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IN SITU INVESTIGATION DURING SPUTTER DEPOSITION OF AG ON ZWITTERIONIC POLYMER FILMS

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While organic electronic devices mainly use organic or organic-inorganic hybrid materials, many electrodes still rely on pure metals due to their unparalleled electrical conductivity. Thus, the polymer-metal interface is crucial for the overall device performance. Studies have demonstrated and established the use of ultrathin metal electrodes for (semi)transparent organic solar cells. The quality of the interface influences the formation of structural defects, which can increase resistance and the likelihood of a short circuit. For research purposes, these metal contacts are typically deposited using lab-scale methods such as thermal evaporation, while industrial manufacturing prefers large-scale methods such as sputter deposition [1,2]. Additionally, zwitterionic polymers have been shown to reduce the work function of metals [3], making them promising candidates as interlayer materials in organic electronic devices. For instance, in inverted organic solar cells, these polymers can serve as interlayers between the electron-blocking layer and the silver electrode. Therefore, understanding the growth behavior of sputtered silver on zwitterionic polymer surfaces is critical. This study investigates the growth behavior of sputtered silver on zwitterionic polymer surfaces using in situ grazing incidence small-angle X-ray scattering (GISAXS) and atomic force microscopy (AFM).

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SIDE-CHAIN AND IONIC FUNCTIONALIZATION OF N-TYPE CONJUGATED POLYMERS FOR OECT APPLICATIONS

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The development of stable n-type organic mixed ionic-electronic conductors remains a central challenge in advancing bioelectronic devices, particularly organic electrochemical transistors (OECTs) [1]. Beyond bioelectronics, they hold considerable promise for a range of applications, including interfacial layers in organic hybrid solar cells [2]. In this context, materials that combine efficient electron transport with ionic conductivity, environmental stability, and compatibility with aqueous media are of particular interest. Here, we investigate the synthesis of n-type conjugated polymers designed to address these requirements through a modular molecular engineering approach.

The polymers core is based on diketopyrrolopyrrole (DPP) and thienopyrroledione (TPD) building blocks, which are copolymerized via direct (hetero)arylation polymerization to yield conjugated backbones. Systematic variation of the side-chain architecture, including linear and branched alkyl substituents as well as oligo(ethylene glycol) chains, is employed to modulate solubility, intermolecular organization, and mixed charge transport. To further enhance n-type stability and introduce ionic functionality, post-polymerization modification is used to incorporate cationic groups. These functional groups are expected to stabilize negative charge carriers on the conjugated backbone, improve ionic transport, and increase compatibility with aqueous environments [3].

By integrating electronic conductivity, ionic mobility, and water-processability within one polymer architecture, this work aims to establish a versatile materials platform for n-type OECTs, related bioelectronic applications, and organic hybrid solar cells. The resulting structure-property relationships will provide insight into the role of side-chain design and ionic functionalization in governing device-relevant performance, thus contributing to the development of more robust and sustainable polymer semiconductors for bioelectronics.

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TOPOLOGY AS A DESIGN PRINCIPLE FOR MOLECULAR EXCITED STATES: FROM ROBUST EXCITONS TO ENTANGLED SPIN QUBITS

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Molecular excited states offer a shared physical basis for robust energy transport and optically addressable spin qubits, linking molecular light harvesting and quantum information through the controlled localization and propagation of excitations. Both rely on excited states that resist disorder and localize or transport on demand, exactly the robustness that topological concepts promise. Yet molecular materials are shaped not only by idealized lattice couplings, but also by charge transfer, long-range interactions, chemical boundaries, disorder, and dissipation. The real question is therefore not whether a molecular system realizes a given topological model, but *when* such a description stays predictive.

We address this with symbolicCI [1], a fragment-based configuration-interaction approach that yields microscopic Hamiltonians for local excitations, radical and charge-transfer states, and, via a Breit–Pauli treatment, spin–spin couplings. In dye aggregates, charge transfer can both overturn a packing-induced topological regime and, at boundaries, mimic topological edge modes that no bulk invariant accounts for. The same framework treats arrays of triplet-radical dyads, where each dyad couples an optically initialized triplet qubit to a stable radical qubit, and the lattice of these entangled two-qubit units can itself carry a topological band structure. This atomistic resolution of the couplings provides the basis for predictive design principles for molecular excited states, from solar light-harvesting to quantum information.

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TOWARDS AUTOMATED SPATIALLY RESOLVED CHARACTERIZATION OF ORGANIC SOLAR CELLS

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Automated, spatially resolved characterization workflows are becoming a key enabling technology for accelerating materials discovery and process optimization in material science. Organic solar cells represent a promising renewable energy technology due to their potential for low-cost, light weight and versatile application while allowing device fabrication via printing methods. Yet, their current optimization strategies are still strongly limited by time and material intensive characterization methods. Current approaches for measuring photovoltaic performance require fabricating individual devices through complex vacuum processes, consuming significant amounts of active, interlayer and substrate materials. Standard procedures evaluate a single set of processing parameters for a single sample. Such single-point measurements fail to capture potential spatial heterogeneities, while averaging spatial properties and neglecting local heterogeneities. As a result, important structure–property relationships can remain hidden, limiting both process optimization and the practical exploration of multidimensional parameter spaces. To address this problem automated and spatially resolved characterization methods can be exploited for fundamental functional material research. If combined with intentional and controlled heterogeneities on samples, high-throughput and material-efficient screening strategies can be enabled. We investigate the possibilities and restrictions on locally resolved I-V and measurements using reversible liquid metal electrodes versus conventional thermally evaporated electrodes. Our automated system employs liquid metal droplet contacts for non-destructive 2D mapping of photovoltaic parameters on PM6:Y12 devices. This methodology offers advantages in material efficiency and measurement reversibility but differs systematically from standard approaches in electrode geometry, contact area determination, and series resistance contributions. We present the comparison of different measurements including comparison to UV/Vis 2D mapping and demonstrate what we can learn from such spatially resolved measurements.

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TOWARDS SUBWAVELENGTH OLED PIXELS

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Next-generation augmented and virtual reality display technologies require a further miniaturization of individual pixels to achieve ultra-high pixel densities. One promising approach is the use of subwavelength organic light-emitting diode (OLED) pixels based on plasmonic nanoelectrodes. In addition to charge carrier injection, these nanoelectrodes function as optical antennas, enabling efficient light outcoupling into the far field while the individual emission properties can be tailored by the antenna geometry. However, when the pixel size is reduced below the wavelength of visible light, sharp nanoelectrode contours dominate the electronic device behavior, resulting in two major challenges: (i) filament formation, leading to rapid pixel degradation, and (ii) non-uniform charge transport and recombination reducing its external quantum efficiency (EQE). To cope with these limitations, we selectively passivate the nanoelectrode periphery with an insulating layer to define the active area of charge injection and recombination by a nanoaperture (see Figure 1). As a proof of concept, we demonstrate efficient hole injection and stable operation of hole-only devices utilizing gold nanoelectrodes. Furthermore, we report, for the first time, light extraction from individually addressable plasmonic OLED pixels with 300 nm × 300 nm dimensions, achieving a maximum luminance of 3000 cd m^{-2} and an EQE of 1% [1].

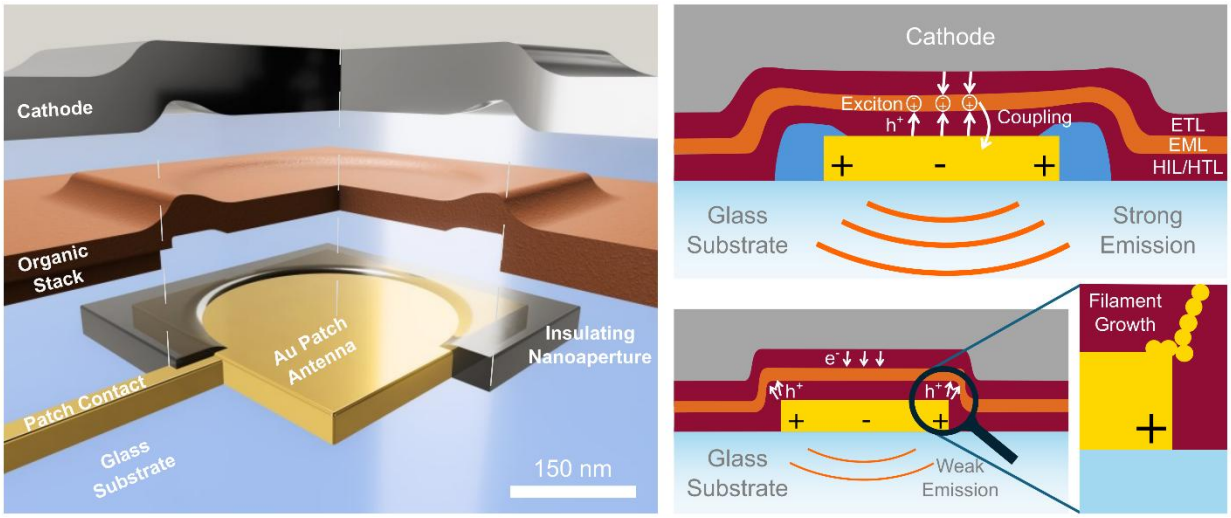


Figure 1: Conceptual nano-OLED pixel design (left), illustrating the passivation of the plasmonic antenna periphery and the central nanoaperture. Cross-sectional scheme with (top) and without (bottom) antenna passivation, indicating the inhomogeneous charge distribution and filament formation in the latter case.

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EXPLORING THE PHASE DIAGRAM OF $FAPbI_3$ USING IN-SITU REFLECTANCE SPECTROSCOPY

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$FAPbI_3$ is a halide perovskite that is particularly promising for solar cells as it has a bandgap neat 1.45 eV and a high absorptivity in the crystalline α-phase. However, the phase stability of $FAPbI_3$ remains challenging, as the photoactive black α-phase is prone to degrade into the inactive yellow δ-phase and can also exhibit a 4H phase that is also not suitable for solar cell applications. To address this issue, we evaluate the temperature- and pressure-dependence of phase transitions using in situ reflection measurements during (hot-)pressing of δ-$FAPbI_3$ powder. We monitor phase transitions parametric in temperature and pressure. We show that the 4H phase is mainly pressure-induced and that the δ to α phase transition temperature of our powder-based thick films decreases with increasing pressure. We are able to derive a phase diagram of $FAPbI_3$ that can serve as guide for device fabrication.

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STRUCTURAL AND OPTICAL INFLUENCE OF LIGANDS ON PEROVSKITE QUANTUM DOTS

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Lead halide perovskite quantum dots (LHP-QDs) exhibit unique size-tunable optical properties, making them promising materials for optoelectronic and photocatalytic applications. Due to their high surface-to-volume ratio, the properties of LHP-QDs are strongly governed by their surface ligands. Here, we show how ligand design can be used not only to stabilize QDs, but also to control their functionality, solvent compatibility, and even their structural properties.

We developed multifunctional ligands that combine strong surface binding, colloidal stability, and a functional molecule. By tethering ferrocene, nitrobenzene, or anthracene moieties directly to the QD surface, we obtain hybrid QD–molecule systems that retain excellent colloidal stability while enabling efficient charge or energy transfer [1]. These hybrid materials provide a versatile platform for tailoring excited-state dynamics through molecular design. Building on this concept, we further achieve ligand-mediated polarity inversion, enabling colloidal stability of LHP-QDs in polar solvents while maintaining a sub-nanometer ligand shell [2]. This expands the range of accessible processing conditions and environments without compromising the optical properties of the nanocrystals. Finally, we show that ligands can also structurally influence the LHP-QDs, highlighting the strong coupling between surface chemistry and the soft lattice.

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OPTOIONIC EFFECTS IN NIOBATE-BASED ELECTRODE MATERIALS

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A critical aspect of solar energy conversion involves the coupling of light-induced generation of charges with their consequent storage. A promising approach toward more efficient solar energy storage are photo-rechargeable or solar batteries, which store light-generated charges directly in an electrode (ideally via photo-intercalation), increase capacity under illumination by activating additional redox processes or accelerate charge carrier dynamics [1,2]. Nevertheless, realizing capacities compareable to established Li-ion batteries has been impeded by the lack of suitable photoelectrodes. In this study, we explore optoionic charge storage effects in established niobium oxides anode materials, which have attracted high interest due to excellent high-rate capacity (up to >200 mAh/g at 10C) [3,4].

The photoelectrochemical response of niobates like $TiNb_2O_7$ or $Nb_{18}W_{16}O_{93}$ are investigated under above-band gap illumination in the context of a standard two-electrode battery configuration. The (photo-)electrochemical responses are measured in half-cells with an optical window for irradiation during (dis-)charge against Li-metal. Influences of photoinduced thermal effects are decoupled from light-introduced effects by investigating the temperature dependence of generated photocurrents and capacity. Thereby, we aim to show how basic materials properties such as band gap and defect concentration can govern the photoelectrochemical response of the electrode and could potentially modulate the performance of solar batteries.

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THROUGH-SPACE VERSUS THROUGH-BOND COUPLING: EFFECTS ON DOWN-CONVERSION IN [2.2]PARACYCLOPHANE-LINKED TETRACENE OLIGOMERS

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In tetracene, the energy of the lowest singlet excited state is comparable to twice the energy of the lowest triplet state, enabling both down-conversion via singlet fission (SF) and up-conversion via triplet-triplet annihilation up-conversion (TTA-UC). The balance between these competing processes is strongly influenced by inter-tetracene coupling, which can occur through both, through-space and through-bond interactions.[1-5]

In a later study, we focused specifically on SF in newly synthesized oligo-tetracenes linked by conjugated [2.2]paracyclophanes (PCP). By varying the substitution pattern and degree of substitution on the PCP linker, we systematically tuned the inter-tetracene coupling. Different connection sites between tetracene and PCP resulted in distinct coupling characteristics: the *pseudo-para* configuration effectively suppresses coupling between tetracene units, while the *pseudo-ortho* configuration promotes through-space interactions due to the closer spatial arrangement. In the PCP-linked tetracene tetramer, both through-space, as in the *pseudo-ortho* configuration, as well as through-bond interactions, *via* the top and bottom phenylene rings, are accessible. These novel oligo-tetracenes were fully characterized using steady-state and time-resolved absorption and fluorescence spectroscopy, focusing on the early stages of SF, namely the conversion of a singlet excited state into a correlated triplet pair.[6]

The present work aims at further investigating the subsequent step of SF: the decorrelation of the singlet-correlated triplet pair.

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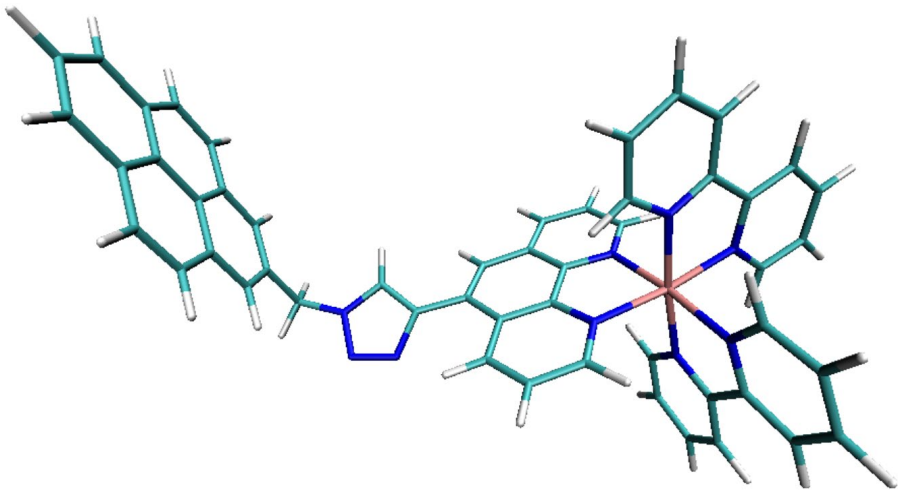
INSIGHTS INTO ELECTRON AND ENERGY TRANSFER IN TRANSITION METAL DONOR-ACCEPTOR SYSTEMS

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Donor-acceptor molecular assemblies consist of covalently linked chromophoric and redox-active units that enable controlled light absorption and subsequent charge or energy transfer, making them versatile platforms for photoredox catalysis and photonics. Their performance is critically determined by the efficiency and competition of photoinduced energy- and electron-transfer pathways, which are highly sensitive to molecular connectivity and geometry. Understanding how through-bond and through-space interactions govern these processes remains a central challenge for the rational design of functional photoactive systems.

In this contribution, we employ time-dependent density functional theory (TD-DFT) to investigate photoinduced electron/energy transfer processes in a series of molecular dyads comprising organic fluorophores (*e.g.*, pyrene, fluorescein, and coumarin) coupled to transition-metal, redox-active Ru(II) or Fe(II)-based units. By systematically varying the bridging motif and connectivity, we elucidate how structural modifications affect electronic communication and the balance between photoinduced electron transfer and resonance energy transfer. Particular emphasis is placed on disentangling *through-bond* and *through-space* processes and assessing how molecular architecture governs the photoinduced reactivity to shine light on the photoinduced electron/energy transfer phenomena.



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SECOND-SPHERE ENGINEERING OF IRON PORPHYRINS FOR ENHANCED CO_2 REDUCTION

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Iron porphyrins are promising molecular catalysts for the electrochemical reduction of CO_2 to CO. Here, we investigate how second-sphere functionalities, including amino groups and crown ether moieties, affect catalytic activity and product selectivity. Electrochemical studies under homogeneous and heterogeneous conditions reveal that the positioning of proton-responsive groups and coordination of alkali-metal ions can significantly enhance catalytic performance. In particular, crown ether-containing derivatives show increased CO formation and turnover frequencies, highlighting second-sphere engineering as a powerful strategy for tuning CO_2 reduction catalysis.

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