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Plenary Lectures

No sustainable energy system without chemical energy conversion

Robert Schlögl[a,b,*]

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Computational design of two-dimensional photo- and electrocatalysts

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Many two-dimensional semiconductors are composed of catalytically active elements, including transition and noble metals. Some of them offer the combination of a suitable band gap for solar light harvesting, band edges suitable for photocatalytic water splitting at neutral pH, high absorbance, large surface area and catalytic activity at the basal plane. Among the most promising materials we propose palladium phosphochalcogenides We are discussing here some noble metal phosphochalcogenides Pd3P2S8 [1] and PdPX, X = S, Se, [2] as interesting candidate materials for photocatalytic water splitting. Being stable in the bulk phase for many years, and with the large surface-to-mass ratio as consequence of their two-dimensional nature, these materials show a high surface area and a very low amount of noble metals which suggests that application is feasible.

With the same argument of noble metal reduction, we explored metallic PtTe. This material (which has been discovered in 1897 as contaminant of silver ore) is metallic as monolayer, which is surprising as most layered metals open a band gap upon exfoliation. We have studied the oxygen reduction reaction in these materials and demonstrate that they outperform the catalytic activity of Pt(111) surface [3].

Finally, I will discuss our latest work on two-dimensional polymers where the π conjugation [4] fosters high charge carrier mobility [5].

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Designing molecular materials for solar-energy conversion

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In this talk I would like to introduce novel molecular materials developed in my group for photovoltaic and photocatalytic applications. In the first part of this talk, high performance fused bislactam-based donor polymers [1] and self-assembling nonfullerene acceptors [2] will be spoken with special emphasis on their aggregation and phase segregation behaviors. Application of them to the organic and perovskite solar cells are to be discussed as well. In the second part of my talk, I will give an overview on our recent efforts to develop organic-based solar driven hydrogen evolution reaction (HER) system. By appropriate ligand engineering, high performance photosensitizers of Ir(III) and Cu(I) complexes were developed to show the outstanding HER performance in combination with Pt colloids. [3,4] We could also develop molecular Pt (II) photocatalyst [5] and self-healable MOF comprising Ir(III) and Pt(II) [6]. Finally, our recent progress in metal-free photocatalyst systems will be discussed.[7]

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Semiconductor nanowires for next generation PV: challenges and sustainability issues

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In views of the scientific evidence of global warming and the responsibility of fossil fuels to this effect, looking for sustainable renewable energy technologies is key. One of the technologies of high potential is photovoltaics. Solar cells not only they can produce electrical power upon exposure to the solar radiation but they can also be used to produce fuels such as hydrogen and methanol.

Semiconductor nanowries, filamentary crystals with diameters tailored in the 100 nm range, exhibit various characteristics that give them great potential for next generation solar cells. Not only they allow a reduction in the amount of material used, but they allow a much more efficient capture of light and carrier collection [1,2]. In this talk, we will review these advantages and also provide a critical view on the challenges we still need to face to render this technology to the marked. Finally, we will also address the issue of using mateirals that contain abundant elements so that these devices can be broadly spread and used.

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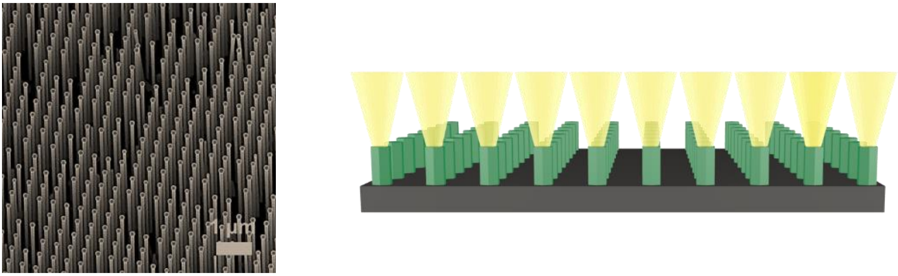

Figure1. Left: scanning electorn micrograph of an array of GaAs nanowires obtained on silicon; **right:** sketch of the capturing of light by the nanowires as optical funnels.

Main-Group Approach toward Functional π-Electron Materials

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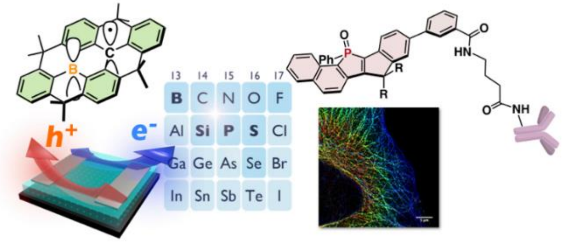
Incorporation of main group elements into π-conjugated skeletons is a powerful strategy to develop new optoelectronic organic materials with unusual properties. Representative design principles are to make use of an orbital interaction between a π-skeleton and a main-group element moiety. Conformational constraint often plays a crucial role to gain an optimal orbital interaction. In addition, this is also important to gain high chemical and/or photo-stability.[1] Based on this strategy, we have so far synthesized various types of functional π-electron materials. In this lecture, we would like to report recent progress in the development of some new main-group element-containing π-electron materials. In particular, we have recently succeeded in the synthesis of a boron-stabilized triphenylmethyl radical, which shows ambipolar charge carrier transport properties.[2] We have also developed new P=O-containing ladder-type dyes, which can show exceptionally high photostability, and thereby can be employed as promising molecules for super-resolution STED imaging.[3]



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Lectures

Tracing single electrons in a disordered polymer host with a single probe molecule

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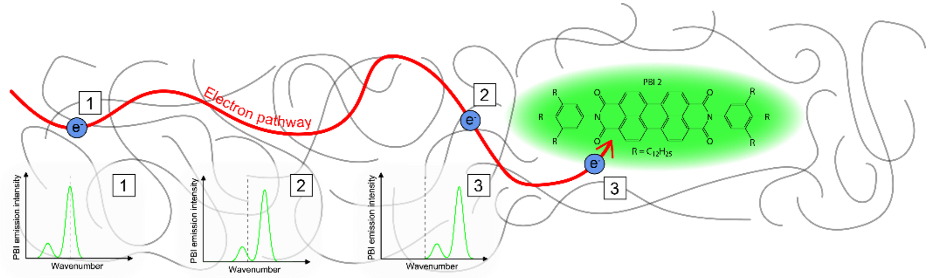
Currently, organic semiconductors enjoy a growing popularity in modern electronics and represent a promising alternative for inorganic semiconductors in the long term. However, due to the significant amount of energetic disorder that is commonly present in these organic devices, microscopic details of the charge carrier transport that lie at the heart of the device performance are unkown. Hence, gaining insights into the underlying charge transport mechanisms in disordered environments is crucial. Based on an earlier work [1], we study the motion of a single charge in the rugged energy landscape of a disordered polymer using a single organic chromophore [2] as probe. In the vicinity of the probe, the electric field of the charge induces a shift of the electronic energy levels of the chromophore that can be monitored as a spectral shift (Stark shift). Performing a proof-of-principle experiment we demonstrate that this approach indeed works, and we will discuss improvements for the data acquisition for optimizing temporal resolution.



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A dynamic view on energy materials: the case of halide perovskites

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Halide perovskites (HaPs) are highly promising energy materials for a range of optoelectronic devices. HaPs are also very interesting scientifically because of the unusual structural dynamics that occur in the material. These include the appearance of complex structural disorder and sizable nuclear anharmonic effects already at room temperature. Since one typically assumes a static ionic lattice displaced from the equilibrium only by harmonic vibrations when describing functional properties of energy compounds, these phenomena challenge our basic understanding of the coupling that occurs between nuclear fluctuations and optoelectronic properties in the material.

In this talk, I will present our recent explorations of the consequences of the unusual structural phenomena in HaPs for their optoelectronic properties. It will be argued that a dynamic view on the functional properties of HaPs can be obtained from theoretical calculations based on density functional theory, molecular dynamics, and tight-binding modeling. These approaches are used to examine the impact of structural dynamics on pertinent device-relevant observables. Consequences of the nuclear fluctuations and anharmonicity in HaPs will be discussed in particular for the charge-carrier mobility and Urbach energy. From this, it will become clear that the impact of the unusual structural dynamics on the optoelectronic properties of HaPs cannot be neglected when understanding these materials microscopically and designing new functional compounds.

Porphyrins and PAHs

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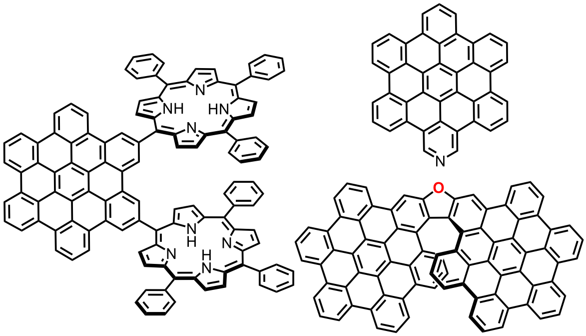
Porphyrins are aptly named “Pigments of life” due to their importance in natural processes such as photosynthesis or oxygen processing. The combination of porphyrins and hexabenzocoronenes and similar polycyclic aromatic hydrocarbons – nanographenes – generates fascinating new architectures. In the lecture, syntheses and properties of new conjugates will be discussed with some emphasis on crystal packing phenomena.



We report on the synthesis, characterization, and properties of some of these novel systems.[1-3] Also, chiral nanographenes will be discussed.[4]

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How does Structure Influence Carrier Mobility in Organic Semiconductors?

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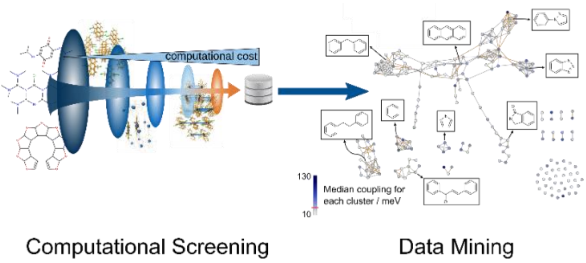
Organic electronics—in the form of field effect transistors, light emitting diodes, or solar cells—are slowly finding their use in everyday consumer devices. So far though, one of the main challenges holding back their widescale adoption are their low intrinsic charge carrier mobilities. Improving these is usually attempted by structural tuning of a promising compound family, thereby relying on intuition, experience, or simply trial and error. While sometimes quite successful, such incremental changes only lead to a local exploration of the potentially vast chemical space of possible molecules, potentially overlooking many interesting materials.
In contrast, modern data mining strategies allow the extraction of general design rules through the systematic evaluation of large compound databases [1]. Starting from an analysis of such a database consisting of >64.000 molecular crystals we evaluate the impact of molecular scaffolds and side groups on the charge transport properties of each crystal contained in our database to reveal statistically reliable, general design criteria [2]. Grouping the molecular
crystals based on the similarity of the scaffolds of the constituent molecules we then visualize the chemical space contained in our dataset as a network to highlight gaps in the experimentally covered range of synthesized organic materials [3]. Thispoints towards promising yet so-far overlooked theoretical and experimental design routes for organic electronics materials.



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Towards nanoscale organic solar cells with controlled morphology

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Conventional bulk heterojunction solar cells are often characterized by a random orientation and/or morphology of the electron and hole conductor at the p/n junction. On the other side, it is kown, that exactly this nanoscale morphology can impact the energy level alignment and consequently exciton separation. Here, we will discuss our steps towards controlling the morphology in nanoscale organic p/n junctions e.g. via careful local engineering of the morphology and electrical characterization of the individual components, in our case the hole conducting polymer P3HT and the small-molecular electron conductor C60. We also discuss our nanoscale electrical measurements of single component systems, namely organic polymer nanofibers [1].

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Energetic Trap Landscape in Perovskite Solar Cells

Philipp Rieder,[a,*] Yinghong Hu,[b] Alexander Hufnagel,[b] Meltem Aygüler,[b] Michiel Petrus,[b] Pablo Docampo,[c] Andreas Baumann,[d] Thomas Bein,[b] and Vladimir Dyakonov [a,d]

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Organolead halide perovskite solar cells have emerged as one of the most promising technologies in thin-film photovoltaics due to their extraordinary increase in performance in only few years, with power conversion efficiencies exceeding 24% already. State-of-the-art devices usually employ mixed cation mixed halide 'FAMA' perovskite, where methylammonium (MA) and bromide is used to stabilize the crystal structure of formamidinium (FA) lead iodide perovskite. The incorporation of inorganic Cesium as well as Rubidium has further proven beneficial for device performance and stability, while simultaneously increasing the structural complexity. In this work, we reveal the impact of Cs and/or Rb on the electronic properties of the FAMA perovskite crystal lattice by directly investigating the energetic landscape of electronic trap states via thermally stimulated current (TSC) spectroscopy on so called triple as well as quadruple cation perovskite solar cells. In TSC, the device is cooled down in the dark well below the activation energy of possible trap states (here: T=30K). Subsequently, trap states are filled with charge carriers created by illumination. After a dwell time allowing charge carriers to relax into the trap states, the solar cell is heated up to 300K with a constant rate, while the current is precisely measured. This current is attributed to charge carriers being thermally released from previously occupied traps in the semiconductor, allowing to draw conclusions about their density and energetic distribution. For the study, the perovskite layer was altered between FAMA, FAMA with 5% of Cs, FAMA with 5% of Rb and FAMA with 5% of Cs as well as Rb in planar type solar cells We found that while Rb had no significant influence on the trap landscape of FAMA, a controlled addition of Cs effectively lowers the trap density in FAMA-based devices, which can be directly linked to the higher performance observed in Cs containing perovskite solar cells.

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Steps of device fabrication: in situ morphology investigations of hybrid solar cells with grazing incidence x-ray scattering techniques

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In the development of non-conventional solar cells not only the achievements of highest power conversion efficiencies and maximum lifetime of devices is of interest. Also the sustainability of the production process of the devices comes into focus. Following this idea, we developed hybrid solar cells with an active layer based on low temperature processed titania and a water-soluble polythiophene [1]. In our approach titania nanoparticles are produced with laser ablation in liquid in order to initiate a functionalization of titania with the polymer for the active layer. The morphology of such layer is investigated with x-ray scattering in grazing incidence [2]. With the applied in situ methods we were able to address individual steps of the production process of devices including the active layer deposition by spray coating and slot die coating, respectively. The final step, the sputter deposition of gold contacts also can be followed with high temporal and spatial resolution. From these studies of individual steps in device fabrication (represented by the icons below) improvements for the processing procedures are derived that allow for a better control of the morphology of the devices.

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Fabrication of porous nanostructures as support for oxygen evolution reaction catalysts with low noble metal loading

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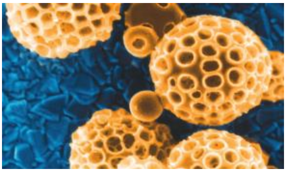
For a large scale application of membrane based electrolyzer technology oxygen evolution reaction catalysts with a significantly decreased noble metal loading are required.[1] Oxidic support materials (TiO_2, SnO_2, etc.) are therefore investigated to achieve higher volume dispersions and an increased stability of the iridium oxide active phase. [2] Macroporous conductive structures could thereby facilitate access of the gas and liquid phases to the catalyst and provide electrical contact to the active phase as well as stabilize it against leaching and sintering. At the same time, they must be stable against oxidation in the electrolyte at the OER potential.[3] The objective is an improved electrocatalytic activity and stability of iridium oxide by an increase of the accessible catalytic surface area and potential novel reactive centers on the surface of disordered ultrasmall particles. The fabrication of conductive macroporous Sb-doped SnO_2 microparticles by a spray pyrolysis reaction and a procedure for homogeneous coating of the support with IrO_x nanoparticles are presented as a model system for further OER catalyst developements.



False colored SEM image of Sb-doped SnO_2 microparticles on F-doped SnO_2 substrate (CeNS calendar image by C. Hohmann from 07/2018)

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Novel Route towards Doped Poly(diketopyrrolopyrrole) Copolymers

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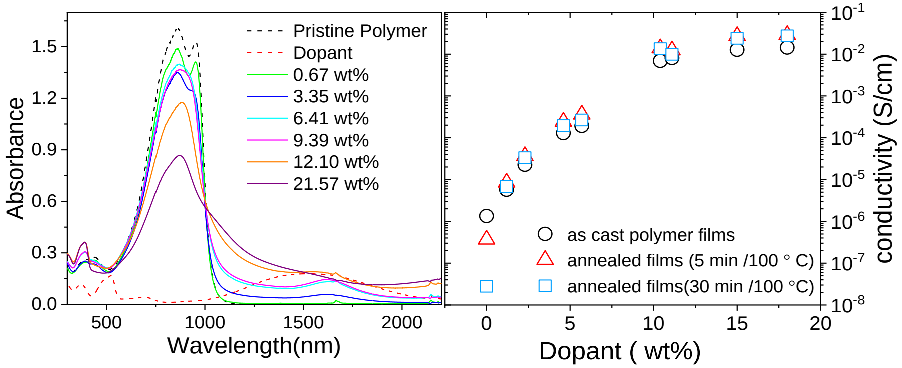
Doped semiconductors are interesting materials as charge extraction layers in perovskite solar cells. In this context, molecular doping is a crucial way to increase the charge carrier concentration and concomitantly the electrical conductivity of semiconducting polymers. The p-type molecular doping of relatively electron rich semiconductor polymers has been extensively studied and F4TCNQ (EA ~ 5.2 eV) has turned out to be one of the most versatile p-type redox dopant for such polymers having IE < 5.2eV. However, most of the high mobility donor-acceptor (D-A) copolymers are known to possess high IE (>5.2eV), which makes them difficult to be doped with commercial dopants such as F4TCNQ. Additionally, F4TCNQ and similar molecular dopants are highly toxic.

To overcome this, in the present work, we have utilized an oxidised hole conductor as a p-dopant to dope a high mobility poly(diketopyrrolopyrrole) copolymer, PDPP[T2]-EDOT by solution processing of host-dopant mixtures. The UV-vis-NIR absorption spectra showed increasing polaron absorption and thin films exhibit four orders of magnitude increase in the conductivity on increasing dopant concentration. Furthermore, detailed time dependent conductivity measurements revealed that the doped films are air-stable and thermally stable. We also provide detailed UPS analysis for the doped films.



Photocatalytic Activity and Light-Tunable Structure of Supramolecular Nano-Assemblies in Solution

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Developing strategies to exploit solar energy becomes more and more important. Inspired by natural systems, it is highly promising to self-assemble building blocks into functional supramolecular entities. In this talk we will present a novel concept to build assemblies in aqueous solution that can act as photocatalysts. [1-3] They consist of ionic polymers and photocatlytically active species of opposite charge such as ionic porphyrins or inorganic clusters. For example, polyelectrolyte-porphyrin nanoscale assemblies exhibit an up to 20-fold higher photocatalytic activity than the porphyrin only and polyoxometallate-macroion asemblies can exhibit an expressed photocatalytic selectivity. A complementary approach is to transfer light energy into nanoscale size and shape changes. [4-6] Basis of the structure formation is an interplay of different non-covalent interactions. We will discuss assembly thermodynamics and structure directing effects. [7]

The concept further has been extended to include metal or semiconductor nanoparticles such as core-shell CdS-ZnS, Ag-doped cadmium sulfide or molybdenum sulfide where electrostatic self-assembly is used to directly create the functional hybrid structures in aqueous solution. [8] Overall, the concept is based on general principles and bears future potential for the design of various complex photoactice nanostructures with tunable functions. [9]

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Towards breaking the barrier to 100% charge transfer

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Chemistry affects almost every aspect of our existence, so that it will be an essential component of solutions in global issues in health, materials, and energy. For this reason, the design and synthesis of novel molecular materials lies at the forefront of transformative research and has game-changing character. A leading example for such shifts in existing scientific paradigms is surpassing the Shockley-Queisser limit, which places an upper bound on solar conversion efficiency for a single p-n junction solar cell at slightly more than 30%, by means of singlet fission (SF) in molecular acenes, the molecular analog to multiple exciton generation (MEG). In an optimal SF process, the lowest singlet excited state of one molecule (S_1) that is positioned next to a second molecule in its ground state (S_0) is down-converted into two triplet-excited states (T_1) each residing on one of the two adjacent molecules. The two triplet states initially form a correlated pair state $^1(T_1T_1)$, which then evolves into two separated triplet states ($T_1 + T_1$). As such, the energetic requirement for SF is $E(S_1) \geq 2 \times E(T_1)$. Shifting the focus to intramolecular SF in dilute solutions rather than intermolecular SF in crystalline thin films enabled the following important breakthroughs:

Firstly, we demonstrated that in a series of pentacene dimers, which were linked by a myriad of molecular spacers, SF takes place with quantum yields of up to 200%.

Secondly, we identified all key intermediates in the SF process, including the formation and decay of a quintet state that precedes formation of the pentacene triplet excitons.

Thirdly, we employed those parts of the solar spectrum, in which pentacene dimers lack absorptions, in non-resonant, indirect excitation of the SF materials via two-photon absorptions or intramolecular Förster resonance energy transfer.

Finally, we succeeded in showcasing the use of up to 200% triplet quantum yields by the realization of 130% carrier multiplication in solar cells for pentacene dimers immobilized onto semiconductors.

Spin related carrier dynamics in $CsPbI_3$ nanocrystals

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Lead halide perovskites demonstrate great potential for optoelectronic applications such as light emitting devices, solar energy harvesting and spintronics. Understanding the spin dynamics of charge carriers in this material could help improving the efficiencies of those applications. Perovskites inhibit large spin-orbit coupling, leading to a large fine structure splitting, which makes both, the conduction and valence band only two-fold degenerate. This allows efficient optical orientation of charge carriers and thus make perovskites an ideal material to study the spin dynamics of photoinduced charge carriers. So far, spin relaxation mechanisms in perovskite nanocrystals have not been investigated in detail. With this study we want to elucidate the carrier spin dynamics and understand the dominant spin relaxation mechanisms on a picosecond timescale in $CsPbI_3$ nanocrystals. We have performed time-resolved differential transmission spectroscopy, where pump and probe beams have circular polarizations of identical or opposite helicity. In this manner, temperature and wavelength dependent measurements have been performed. We compare our experimental data to theoretical models and discuss possible microscopic origins of spin scattering.

Magnetic Field Effects in Rigidly Linked D-A Dyads: Extreme On-Resonance Quantum Coherence Effect on the Charge Recombination

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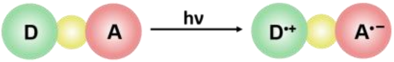
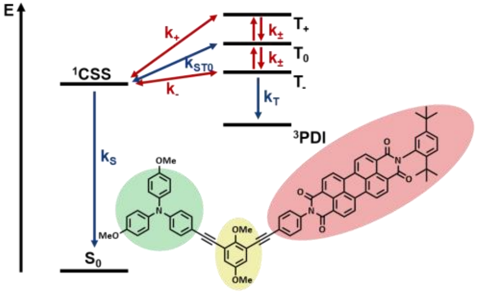
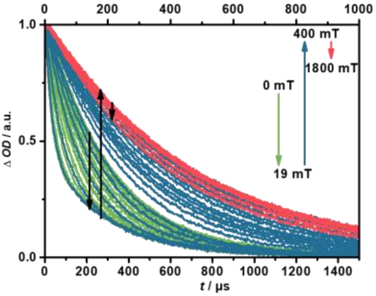
Rigidly linked radical pair (RP) systems formed by photoinduced charge separation are highly interesting for solar energy conversion, but also represent ideal model systems for principal studies in experimental and theoretical spin chemistry. Depending on the ratios of the rate parameters of the general RP reaction scheme, a variety of phenomenologically quite different magnetic field effects (MFEs) can ensue. Here we report on a striking MF dependent charge recombination in non-polar solvents such as toluene. At magnetic fields, off-resonance by more than about ±5 mT, recombination to ^{3}PDI is purely monoexponential, while the decay is biexponential and much faster in the resonance region. Description by a classical kinetic approach based on an extended Hayashi-Nagakura model works well outside the resonance region, whereas only a quantum dynamical calculation can account for the kinetics at resonance. [1, 2]







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Anomalous exciton diffusion in polymers of varying length, observed by EEI2D spectroscopy

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Exciton transport and interaction in molecular aggregates and polymers is one of the key processes in solar light harvesting. While the initial ultrafast excitation dynamics proceeds in a delocalized, wavelike fashion, the subsequent exciton transport is commonly described by a normal diffusion, characterized by the exciton diffusion coefficient and diffusion length. In this work we use our newly-developed exciton-exciton interaction two-dimensional (EEI2D) spectroscopy[1], in combination with microscopic theoretical modelling, to study exciton dynamics and annihilation in squaraine copolymers of varying length. By directly probing interacting exciton pairs, we observe the transition from wavelike to diffusive exciton motion, dependent on the exciton delocalization length relative to the polymer size. Contrary to the common assumption, we find that the exciton diffusion has anomalous, sub-diffusive character, indicating trapped excitons. Our results imply that to characterize the exciton transport in conjugated systems, normal diffusion should not be taken for granted, but the diffusion character should be determined. For this task, the EEI2D spectroscopy is a well-suited technique.

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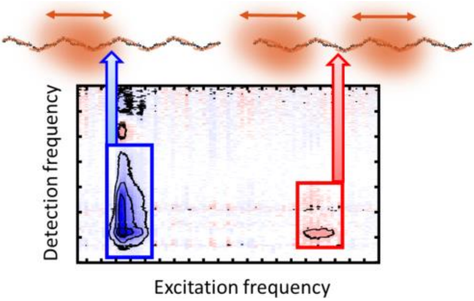

A Solvent free Route for Halide Perovskite Film Processing Based on Pressure Treatment of Perovskite Powders

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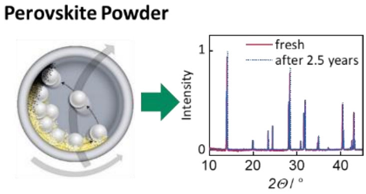
Even though hybrid perovskites have undergone a remarkable development within the last years, state of the art processing approaches such as solution processing or evaporation suffer from an intrinsically high complexity, as the actual perovskite crystallization and its film processing happen simultaneously and are inextricably interconnected.

Here we present an alternative, entirely dry processing approach, which decouples perovskite crystallization and film formation, by using readily prepared perovskite powders and produce films by appropriate mechanical pressure treatment. We show how a mechanochemical synthesis approach by ball milling allows us to produce a wide range of phase pure and exceptionally stable hybrid perovskite powders with a high flexibility in processing and address the impact of milling parameters on the powder properties. Using these powders, we demonstrate how the used pressure and the powder microstructure, i.e. particle size and stoichiometry affect the mechanical stability, compactness and surface roughness of the pressed layers. We further address how specific temperature treatment during the pressing step can improve the properties of the pressed layer, and show their capability to be used in perovskite based optoelectronic devices, such as X-Ray detectors.



Organic semiconductors and hybrid materials for optoelectronics

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This lecture will give an overview of our recent activities in the field of charge generation and light emission from organic semiconductor heterostructures as well as lead halide perovskite nanocrystals.

In the first part, we will address the important role of intermolecular charge transfer states at organic donor-acceptor interfaces and demonstrate how morphology and molecular properties affect their density of states [1]. We will further discuss energy losses in the context of reciprocity between LEDs and solar cells [2].

The second part will deal with the emerging class of lead halide perovskite nanocrystals. In particular, we will demonstrate how the orientation distribution of their optical transition dipole moments can be manipulated by size and shape and discuss the potential for improved light outcoupling from such nanocrystal LEDs [3,4].

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Ultrafast spectroscopy of charge and structural dynamics in hybrid perovskites

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Femtosecond laser sources have generated a wide range of tools to study electronic state properties, excited state populations and structural dynamics in functional materials. Unique insights are gained into the working mechanisms of semiconductor materials for optoelectronics, which are crucial to advance device efficiencies and solve the global energy challenge. Scientifically, the connection between material structure and electronic properties is a fundamental question, for which mainly the limits of ordered (crystalline) and disordered (amorphous) semiconductors have been studied.

Recently, the class of metal-halide perovskites have emerged as an intermediate semiconductor type, in which the soft-crystalline material structure leads to unexpected excited state dynamics, and for which the underlying physics remain unexplored. Unusually strong spin-orbit coupling was predicted to introduce Rashba-type state splitting in the electronic band structure of these materials, which is expected to affect recombination dynamics and spin-populations. It remains an open question, how dynamic changes in the material structure and electronic state populations, in combination with Rashba effects, control application-relevant electronic state nature and relaxation.

In my talk I will present how we use advanced optical spectroscopy to study the dynamics of optically-excited electronic state populations, crystal structure and spin in functional hybrid perovskite semiconductors on ultrafast timescales. I will present results on layered and bulk metal-halide perovskites of varying dimensionality, for which I will discuss how the crystal structure and composition controls the properties and recombination of electronic states, and how these can enable highly-efficient optoelectronic devices and novel functionality.

Bismuth Impurities and Negative Capacitance in Lead-Halide Perovskite Solar Cells

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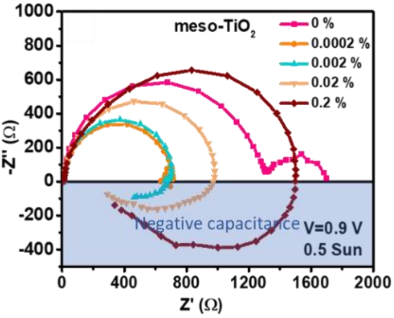
In this contribution we investigate the role of impurities in perovskite solar cells. We deliberately introduce small quantities of bismuth (10 ppm to 2%) into mixed cation mixed anion perovskite films [1]. We observe that the open-circuit voltage decreases systematically with impurity concentration even in the ppm regime. This strong defect intolerance against Bi impurities comes along with reduced electroluminescence yields and charge carrier lifetimes obtained from transient photoluminescence experiments. Calculations based on molecular dynamics and density functional theory predict delocalized (0.16 eV) and localized deep (0.51 eV) trap states dependent on the structural arrangement of the surrounding atoms. Sensitive measurements of the photocurrent (by FTPS) and surface photovoltage (SPV) confirm the presence of tail states.

Interestingly, the addition of Bismuth provokes a negative capacitance (see figure), which has been observed several times but remained a puzzling phenomenon. We reveal the origin of this phenomenon and propose a model based on modified electronic charge injection as a response to slowly moving ionic charge in the perovskite film [2].



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Multimetallic nanoparticles in catalysis: electronic structure insights and challenges

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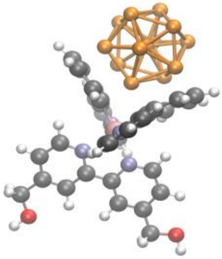
Developing improved catalysts is an important aspect of "Green Chemistry". Electronic structure theory can help to understand experimental findings and thus hopefully will be able to guide, e.g., the development of new photocatalysts. However, real-world systems are often of a complexity and size that seriously challenge existing electronic structure methods. In this contribution we will first discuss examples of how combining different metals can enhance catalytic activity [1,2] and that there is hope that such synergistic effects can lead to new photocatalysts, e.g., for water splitting [3]. In a second step we will then report and discuss efforts to understand such systems based on electronic structure theory. We will point out the urgent need for theoretical approaches that are first-principles, i.e., non-empirical, and accurate, yet at the same time computationally efficient enough to be able to treat large, experimentally relevant systems. A newly developed density functional that appears very promising in this respect will be presented [4].



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A New Synthetic Approach towards Planar and Bowl-Shaped Polycyclic Aromatic Dicarboximides

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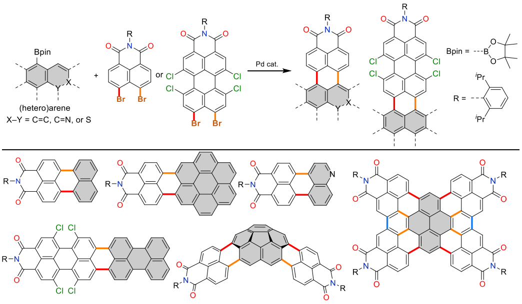
Research in polycyclic aromatic hydrocarbons (PAHs) has diverged in recent years in terms of functionalization and variation of shape and size of their scaffold. Among many functionalized PAHs, polycyclic aromatic dicarboximides (PADIs) are a valued class of functional materials due to their n-type semiconductor properties and suitable functionality which allows them to form suplamolecular assemblies. However, synthesis of PADIs in many cases requires pre-formation of a core PAH scaffold. Therefore, we have been engaging in development of a new synthetic method that can be applied to afford PADIs with structural and topological diversity.[1] Here we present our recent accomplishments on the synthesis of planar and bowl-shaped PADI [1,2] (see below) using palladium-catalyzed annulation reaction between aryl boronic acid pinacol esters and dihalo-napthalene dicarboximides. The reaction proceeds via a Suzuki–Miyaura and direct arylation cascade and affords PADIs with planar and bowl-shaped scaffolds as well as heteroatom-doped PADIs.[3] Our current results on the expansion of reaction scope and molecular properties of unique planar and bowl-shaped PADIs will also be presented.



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Simulation of Large Photo- and Electroactive Systems

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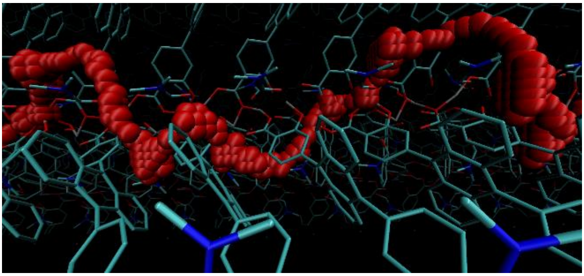
Realistic quantum mechanical simulations of technically important aggregates, polymers and nanoparticles require that many thousands of atoms can be treated, [1] for both ground and excited states. Furthermore, amorphous systems can best be simulated in periodic calculations that use a repeat unit of many thousand atoms [2] to give a pseudo-amorphous structure. Our preferred tool for such calculations is semiempirical molecular-orbital (MO) theory, although we often use density-functional theory (DFT) to obtain geometries for calculatons of spectra. Alternatively, QM calculations may be based on ensembles of snapshots from classical molecular-dynamics (MD) calculations in order to obtain time-averaged spectra or transport properties.

An example of such calculations for molecular systems is the investigation of the effects of chromophore multiplication in molecules substituted with several pentacene moieties. [3] Covalent and metal-organic frameworks (COFs and MOFs, respectively) represent "soft" molecular crystals, in which dynamics are important, so that the effect of srtructural flexibility must be taken into account. [4] The figure shows a calculated hole-transport path in a MOF.



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Posters

Synthesis and characterization of lead-free double perovskites

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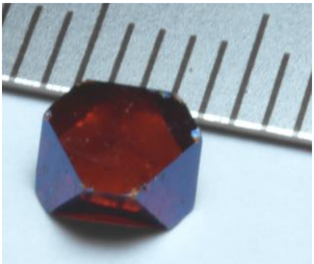
As conventional perovskite solar cells contain lead and therefore suffer toxicity as well as stability issues [1], finding alternative lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, $Cs_2AgBiBr_6$ and $Cs_2AgBiCl_6$ crystals have been synthesized, permitting a detailed characterization of the optical properties of these materials. The films have been characterized using steady state and time-resolved optical spectroscopy. The morphology and quality of the as prepared crystals has been evaluated using scanning electron microscopy and X-ray Diffraction.

It has been found that crystals of both double perovskites can be grown from solution. Furthermore, we observed photoluminescence of both perovskites in the visible region. Additionally, we observed long lifetimes up to 700 ns for $Cs_2AgBiBr_6$ single crystals, measured by time resolved photoluminescence. Due to the encouraging optical properties and the straightforward growth processes we propose $Cs_2AgBiBr6$ to be a promising candidate for the application in lead-free perovskite solar cells.



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Thermoelelectric Characterisation of n-Type Doped C_{60} Thin Films

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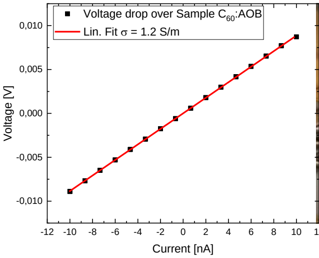
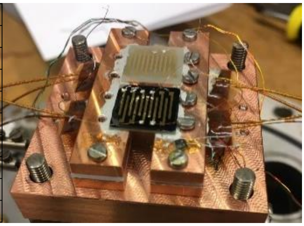
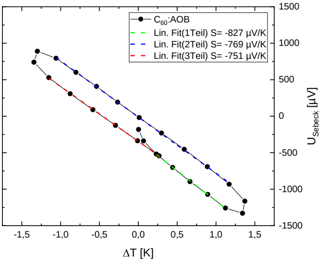
The efficiency of thermoelectric applications is determined by their figure of merit $zT = \sigma S^2/\kappa$ where σ refers to the electrical conductivity, *S* to the Seebeck coefficient and the thermal conductivity is denoted by *κ*. Therefore, it is a key challenge to find p- and n-doped semiconductors with high *zT* values. A promising class of materials to achieve the desired properties and, thus, to be implemented in future thermoelectrics is represented by organic semiconductors, as they intrinsically feature low *κ* values by their weak van der Waals interactions and high Seebeck coefficients. Furthermore, their electrical conductivity σ can be significantly increased by doping. However, the search for stable n-type doped molecular layers turns out to be challenging. Fullerene C_{60} has proven a promising host, as it can be n-doped by various donor materials, including air-stable compounds like acridine orange base (AOB) [1]. Using the material combination C_{60}:AOB as starting point, we analyse the thermoelectric characteristics as function of dopant concentration and temperature. The transport properties are discussed in relation to both the underlying thin film morphololoy estimated by AFM and X-ray diffraction as well as the respective doping efficiency. The results are discussed in view of implementing n-doped fullerene layers in thin film thermoelectric generators.



I-V curve of a doped C_{60} thin film



Setup for resitance and seebeck measurements with reference substrate (up) and exemplary sample (bottom)



Seebeck measurement curve of n-type doped C_{60} thin film

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Pressure dependence of bidirectional, buffer-mediated Proton-Coupled Electron Transfer

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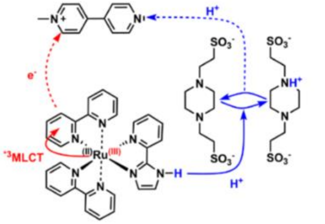
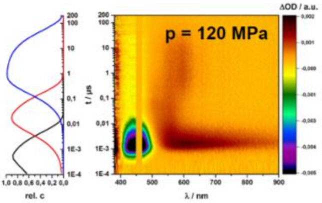
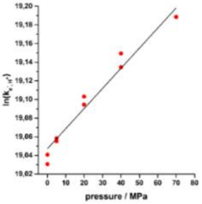
Excited state Proton-Coupled Electron Transfer (PCET), activated upon optical excitation, is a promising tool for solar energy conversion, energy storage, small molecule activation and catalysis.[1,2] As the combination of proton- and electron-transfer is likely to occur either stepwise or concerted, involving differently charged intermediates and activated complexes, the solvation-sphere and volume strongly depends on the underlying mechanism. Thus, the mechanism of bidirectional, light induced PCET from, for example, $[Ru(bpy)_2pyimH]^{+2}$ to N-methyl-4,4'-bipyridinium,[3] involving a buffer as proton mediator, was probed by means of pressure dependent transient absorption spectroscopy, NMR, and cyclic voltammetry as well as complemented by molecular modelling. The negative activation volume of $\Delta^{\ddagger}V^{*} \approx -4\ cm^{3}mol^{-1}$ for PCET in the excited state points towards a concerted mechanism active.







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Iridium oxide nanoparticles on inverse opal antimony doped tin oxide microparticles as highly active oxygen evolution catalysts

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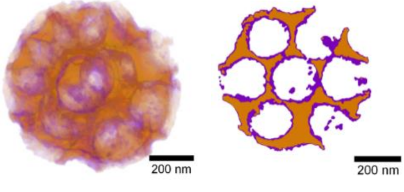
Water splitting for hydrogen production has been recognised as promising solution for chemical energy storage and energy conversion with regard to renewable energy sources. With electrocatalysts playing an important role for water splitting, iridium was shown to be one of the most promising candidates featuring high activity and stability – however, at the expense of a high price and limited availability of iridium.

We present a multistep synthesis procedure for the homogeneous coating of highly porous conductive oxide microparticles, loaded with remarkably low amounts of iridium nanoparticles for water oxidation applications. Macroporous Sb:SnO_2 (ATO) microparticles with defined pore size, composition and morphology were obtained using polymer-based templates in an ultrasonic spray pyrolysis procedure. These particles can be used as a conductive support for electrocatalysts featuring high surface areas and porous morphology. As active catalytic material, IrO_2 nanoparticles ~2-3 nm in diameter were synthesized by a solvothermic reduction of an IrO_x-colloid suspension in the presence of the ATO microparticles to obtain homogenously covered composite particles. Electron tomography was performed to verify the complete coverage of IrO_2 inside and outside the porous ATO particles. Further, the amount of the used active material was calculated based on the density of the materials, size distribution and tomographic datasets to optimize the amount of the rare-metal catalyst. A remarkably low Ir bulk density of ~0.08 g cm^{-3} for this supported oxide catalyst architecture with 25 wt% Ir could be determined. This highly efficient oxygen evolution reaction (OER) catalyst reaches a current density of 63 A g_{Ir}^{-1} at an overpotential of 300 mV vs. RHE, significantly exceeding a commercial TiO_2-supported IrO_2 reference catalyst under the same measurement conditions.



A Kinetics-Based Computational Catalyst Design Strategy for the Oxygen Evolution Reaction on Transition Metal Oxides

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Aiming to extend over prevalent thermodynamical models, we present a catalyst design strategy for the oxygen evolution reaction (OER) at transition metal oxide (TMO) surfaces that explicitly considers aspects of the reaction kinetics. This strategy is based on recent insights from evaluating a large number of doped active sites on three different surface terminations of cobalt(II,III) oxide (Co_3O_4) [1] and previous quantum mechanical studies of the reaction on pure Co_3O_4 [2,3]. On this basis, we adapt existing Brønstead-Evans-Polanyi relationships to achieve an accurate description of the two-step nature of the rate-limiting water addition step in the OER. This reveals that the electrochemical and nonelectrochemical pathways of water addition are kinetically equivalent under certain conditions. It also yields a simplified kinetic model to derive a generalized expression for the catalytic activity. We use this model to formulate design criteria for optimal catalytic performance, which pose structure-sensitive and electrode-potential-dependent restrictions for the oxidation potentials of the metal centers involved in the reaction. The kinetics-based design strategy as well as these design criteria are expected to be transferable to other TMOs and similar electrocatalytic systems dominated by kinetic barriers.

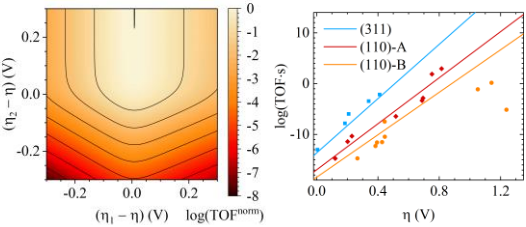

Fig. 1: Representative dependence of TOF on the oxidation potentials η1 and η2 of the metal centers involved in the OER (left). Maximum attainable TOF at a given electrode potential η for three different active site structures and various calculated sites. Figures adapted from Reference [1] (right).

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TiO_2 corrosion protection layers by atomic layer deposition

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Many photoactive semiconductors face instabilities in the harsh chemical environments required for water splitting reactions. A promising approach to address this issue is the formation of protective layers that physically separate the photoelectrode from the electrolyte but at the same time facilitate selective charge carrier transport and light transmission. To achieve the combination of properties required for effective protection of photoelectrodes, atomic layer deposition (ALD) plays a key role due to its ability to create highly conformal thin films with atomically precise layer thickness control. Recently, TiO_2 thin films were proven to enhance the lifetime of established photoanode materials without significantly diminishing their performance [1]. In this context, a defect mediated charge carrier transport through the TiO_2 was proposed. To further investigate and control this phenomenon, we deposited TiO_2 films onto the model substrate silicon by thermal, as well as plasma-enhanced ALD, and compared both the optoelectronic and electrochemical properties of the resulting films. Insights into the role of mid-gap states within the protection layer on functional properties are obtained by evaluation of (photo)electrochemical characteristics alongside advanced probes that are sensitive to defects, such as photothermal deflection spectroscopy, surface photovoltage spectroscopy, and variable angle spectroscopy ellipsometry. In the future, these approaches will be extended to other photoanode and photocathode materials to create highly efficient and stable photoelectrochemical systems.

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Temperature-Dependent Ambipolar Charge Carrier Mobility in Large-Crystal Hybrid Halide Perovskite Thin Films

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Perovskite-based thin-film solar cells today reach power conversion efficiencies of more than 22% [1]. Methylammonium lead iodide (MAPI) is prototypical for this material class of hybrid halide perovskite semiconductors and at the focal point of interest for a growing community in research and engineering. Here, a detailed understanding of the charge carrier transport and its limitations by underlying scattering mechanisms is of great interest for the material's optimization and development. We present an all-optical study of the ambipolar charge carrier diffusion properties in large-crystal MAPI thin films in the tetragonal crystal phase from 170 K to room temperature [2]. We probe the local material properties of individual crystal grains within a MAPI thin film and find a steady decrease of the ambipolar charge carrier diffusion constant with increasing temperature. From the resulting charge carrier mobility, we find a power law dependence of $\mu \propto T^{m}$ with $m = -(1.8 \pm 0.1)$. We further study the temperature-dependent mobility of the orthorhombic crystal phase from 50 to 140 K and observe a distinctly different exponent of $m = -(1.2 \pm 0.1)$ [2]. Furthermore, the phase transition itself is in the focus of our interest, closing the gap of our measurements between tetragonal and orthorhombic phase. As a result of our more detailed spectroscopic and microscopic measurement techniques, we demonstrate the local behavior of single crystals within thin films during the phase transition.

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Passivation of Defects with Organic Ammonium Salts for Efficient and Stable $MAPbI_3$ Perovskite Solar Cells

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The high efficiency as well as the easy solution and low temperature processability of perovskite films makes them an attractive platform among photovoltaic technologies. However, the polycrystalline property of low temperature solution processed perovskite films inevitably leads to the presence of crystallographic defects at perovskite surfaces and grain boundaries (GBs).[1] For example, the methylammonium cation (MA^+) in $MAPbI_3$ can be easily released as methylammonium iodide from the 3D lattice under solar cell operating conditions.[2] This release of MA^+ further causes the generation of different types of defect such as under-coordinated Pb and Pb-I antisite defects.[3] These defects deteriorate the photovoltaic performance and stability.[4] To address this issue, organic small molecule components, in their neutral and salt forms, are applied between active layer ($MAPbI_3$) and hole transporting layer to passivate these inevitable defects at GBs and interfaces to obtain more stable and more efficient solar cells. After treatment, over 10 % PCE enhancement is observed compared to the reference, mainly due to the improved V_{oc} and FF. These results demonstrate the need for the molecular design of new passivators to make perovskite solar cells more promising and reliable for industrial applications.

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Study of Organic Colloidal Nanoparticles Synthesis

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Between the technologies available for alternative energy production, solar energy harvesting is one of the most researched and invested topics, which alone in 2017 was responsible for producing more than one third of all the net power capacity between the renewable power sources[1]. Among the energy harvesting technologies available, the organic photovoltaics hold the promise of low -cost renewable energy source, with appealing properties such as light weight, flexibility, solution processable and possibility of application over large areas[2]. Although bulk heterojunctions (BHJ) systems are the most successful employed method for organic solar cells construction, they require high volumes of hazardous solvents for processing, which could cause a high impact on the environment, presenting a serious difficulty for using this approach for upscaling. A possible solution lies in the organic solar cells made from water based dispersions of polymer nanoparticles (NPs), which not only require lower amounts of solvents but also enable the possibility of ink formulation and the consequent separation between the active layer blend formation and its integration into different processes, making them a very attractive topic for research[3]. Although there are several methods to produce organic nanoparticles, such as the ones based on changes of solubility, mini-emulsion and reprecipitation, an in depth systematic study about the process of the formation and morphology control of the nanoparticles is still not available. Therefore, a stopped flow system which enables simultaneously precise mixing, temperature control and *in situ* monitoring of changes in absorbance (ABS) and photoluminescence (PL) as the nanoparticles are being formed, plays a crucial role for research in the NPs formation and morphology, which is essential for the development of the photovoltaics field.

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Direct probing of solvent-modulated photoisomerization reactions via broadband ultrafast transient absorption spectroscopy on a merocyanine dye

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Merocyanines are an important class of functional dyes that can be used in a wide range of applications in fields, such as, organic semiconductors [1], non-linear optics [2], and chemical analysis as well as in biology and medicine as probes and markers. [3,4]
Herein, we report on the direct probing of solvent-modulated photoisomerization reactions of a merocyanine dye [5], utilizing broadband ultrafast transient absorption spectroscopy which enables us to determine and identify characteristic lifetimes of exicted states. We complemented our experimental data by quantum chemical calculations to assist in identifying the photoinduced key rotational processes leading to structural changes of the merocyanine backbone and therefore, characteristic spectral signatures in transient absorption.

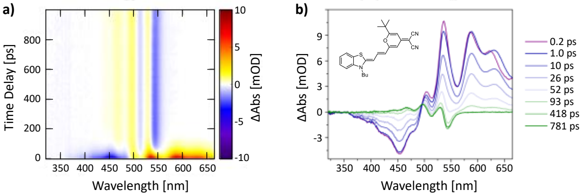

Fig. a) Broadband ultrafast transient absorption in methylcyclohexane, $\lambda_{ex} = 540$ nm and b) corresponding selected spectra at various time delays.

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CO_2 reduction reaction on Cu_2O-oxide derived catalyst, a novel case of oscillations

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CO_2 reduction reaction (CO_2RR) has attracted much attention in electrocatalysis[1] since it allows the synthesis of more valuable chemicals and fuels, whichcan be classified as solar fuels [2] if solar power sources are used. In this process, CO_2 is reduced to molecules like CO, formic acid/formate, methane and/or C_2 hydrocarbons, depending on the catalyst [1] Among all the regular catalysts, Cu stands out as it is the only electrode material catalyzing C-C coupling during CO_2RR.[1,2] However, the product selectivity during CO_2RR on Cu is quite poor.[2] One way to increase the selectivity is to use so-called oxide derived (OD) catalysts,[3] materials that initially are oxides, but in operando conditions become metallic, though the resulting Cu_2O-OD material having with different structural proprieties than bulk Cu We tested the electrochemical Cu_2O-OD response to CO_2RR using K_2CO_3 electrolyte saturated with CO_2. During this investigation, we could observe and interesting behavior during step potential application, the I-t profile being non-monotonous and exhibiting oscillations of the steady-state current after about 1000 s. When the current is kept constant at a level close to the minimum of the I-t curve under potential control, potential oscillations are observed. These facts show that the reaction features non-linear dynamical properties which have not been reported in the literature until now but might be exploited to increase the selectivity of CO_2RR.

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Energy level alignment and charge transport at the semiconductor-protoporphyrin IX-interface

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Efficient photocatalytic conversion of carbon dioxide to solar fuels presents an attractive option to reduce the problem of energy storage present in today's renewable energy technology. By anchoring molecular catalysts on semiconductor surfaces and therefore combining approaches of heterogeneous and homogeneous catalysis, one might be able to profit from advantages of both, leading to enhanced efficiency and stability.

In order to gain more information specifically on the energy level alignment and charge transport between catalytically active molecules and semiconductor surfaces, a simple model system containing a protoporphyrin IX (PPIX) monolayer deposited on different semiconductor substrates via Langmuir-Blodgett deposition is investigated. Monolayer morphology as well as molecular packing density are studied using atomic force microscopy and surface pressure isotherms, indicating a closely packed monolayer with a slightly tilted orientation on Silicon and Gallium Nitride surfaces. Photoluminescence (PL) studies of PPIX monolayer deposited on Silicon and Aluminum Gallium Nitride surfaces with varying Aluminum to Gallium ratio indicate a strong dependence of the PL intensity on the band gap of the underlying substrate and excitation wavelength. Shorter excitation wavelengths and higher electron affinities of AlGaN substrates yield lower PL intensity. That gives rise to the assumption that electrons in excited molecular states are transferred to the substrate's conduction band, if the excited electron has sufficient energy compared to the conduction band minimum. This leads to a quenching of the luminescence in this model system and could lead to a decrease in efficiency for a photocatalytically reducing device, highlighting the necessity of matching the choice of the semiconductor support to the catalytic molecule.

A Direct Inversion Approach to Local Permittivity

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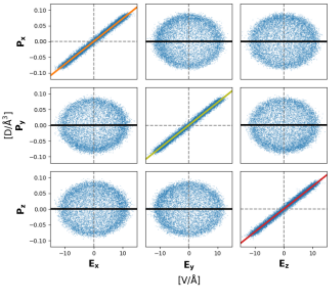
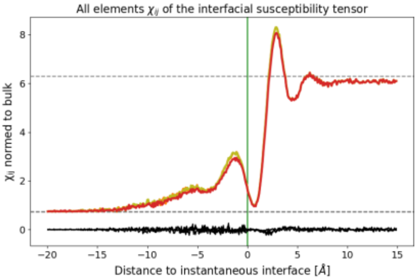
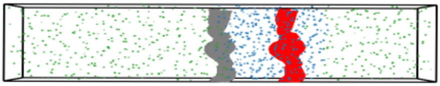
Implicit solvation models are widely used in electronic structure simulations of catalytic reactions in condensed phases. This is due to the fact, that in such complex systems quantum-classical embedding schemes often present the only viable methodology of simulation due to their simplicity and advantages regarding computational cost [1,2]. These approaches only model a solute region explicitly while the interaction with the gross part of the solvent is coarse-grained into a continuum dielectric response, instead of considering individual solvent molecules. This dielectric response described by the solvent static dielectric permittivity ε, often enters such models as a free parameter which deviates, sometimes drastically and anisotropically, from its isotropic bulk value in vicinity of the solute. We present a possible procedure relying on a direct comparison of instantaneous polarization and Maxwell field for neutral and spatially compact subdomains. In this way, we gain access to the spatially resolved full-rank static permittivity tensor while also avoiding an artificial, a posteriori introduction of boundary conditions for phase separation in interfacial systems.







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Photobase Effect in Photocatalytic Activity of Carbon Dots

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Carbon dots (CDs) are a versatile nanomaterial with attractive photoluminescent and photocatalytic properties. Their complex internal structure, considered to comprise sp^2-hybridized domains embedded in an amorphous sp^3-hybridized matrix, results in an intricate interplay between the constituent parts with multiple charge and energy transfer pathways determining the photocatalytic properties.[1,2] In effect, the mechanism of the photocatalytic hydrogen generation with CDs remains a subject of debate. Here we demonstrate that the mode of nitrogen inclusion in the CDs within the aromatic domains controls the charge transfer and separation and thereby the photocatalytic activity for water reduction. [3,4] Furthermore, we propose that the photobasic effect, that is the abstraction of a proton from water upon excitation of CDs by light, facilitates the photoexcited electron transfer to the proton. In this context, we studied the effect of controlled inclusion of photobasic molecules into CDs which resemble the molecular moieties found in photocatalytically active CDs. We show that such addition strongly increases the hydrogen generation. Ultrafast spectroscopy measurements corroborated these findings, revealing the dynamics of the relevant electron and excited state proton transfer processes. The study demonstrates the critical role of understanding of the structure and dynamics of the CDs in designing the materials with improved photocatalytic efficiency.

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GaP nanowires: Photocatalytic cathodes for Carbon (IV) oxide reduction

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Increasing CO_2 concentration in the atmosphere is believed to have a profound impact on the global climate. One of the ways to reverse this negative impact is developing effective strategies to capture and utilize CO_2 from the atmosphere. Among several available strategies, CO_2 reduction via the electrochemical or photochemical approach is particularly attractive since the required energy input can be potentially supplied from renewable sources such as solar energy [1]

Compared to other available semiconductors, gallium phosphide (GaP) is considered a highly promising photocathode material for solar-fuel conversion. Its high conduction band edge allows it to reduce not only water into hydrogen but also CO_2 into chemical fuels [3]

However, the conventional planar geometry from a single crystalline wafer poses an obstacle to exploring the potential of GaP fully, since in the planar geometry most of the photons absorbed by GaP do not fall within the charge collection layer, as is required for an efficient photo electrode. [3] Recent progress indicates that this issue could be solved when the photo electrode is composed of semiconductor micro wires [4]

We have synthesized GaP nanowires using functionalized multi-walled carbon nanotubes (CNTs) as substrates by the reaction between gallium vapor and phosphorus vapor inside a tube furnace system. The as synthesized nanowire Gap-CNTs were characterized by Field emission scanning electron microscopy (FESEM), high resolution transmission electron microscopy (HRTEM) and X-ray diffraction (XRD). We present our findings on the exploration of these nanowires deposited on glassy carbon surfaces and silicon wafers as effective photocathodes for CO_2 reduction in acidic medium.

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Plasmonic effects in photoelectrochemical systems

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The field of plasmonics has been extensively researched and used for a wide variety of applications, such as cancer treatment in biological tissue, field enhanced Raman spectroscopy and heterogenous catalysis. Especially in the field of energy conversion and storage, which is now more than ever necessary to address the energy and climate challenges, the utilization of plasmonic effects seem to be a promising possibility to tune and enhance catalytic properties of (photo-)electrochemical systems.

There are several influences that plasmonic effects can have on chemical reactions, e.g. plasmonic heating [1], nano bubble creation [2], field coupling to the reactants [3] or hot carrier injection [4]. In this work we investigate plasmonically active arrays of gold nanosquares with high aspect ratio on silicon substrate, which are created by lift-off nanoimprint lithography [5], as an exemplary photoelectrochemical system regarding their catalytic properties and the ability to utilize plasmonics for photoelectrochemical applications.

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Out-of-the-box implicit solvation at dielectric interfaces

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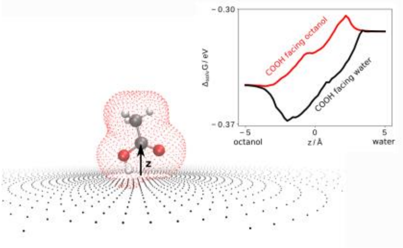
Implicit solvation models are widely used to incorporate solvent effects into molecular simulations. Instead of explicitly sampling solvent degrees of freedom they approximate the solvent as a structureless dielectric continuum. Although generalizations for heterogeneous environments have existed for some time, only recently the first of these were included as out-of-the-box functionality in some electronic structure software packages [1]. We modified the multipole expansion (MPE) model [2] to account for dielectric interfaces, specifically focusing on the electrostatics of mutually interacting dielectric media. Non-electrostic contributions to the free energy are treated with a simple linear model, fitted to experimental free energies of solvation in the respective media. Our model will be released in a future version of the FHI-aims package [3] and requires only minimal user input. We demonstrate its efficacy for small organic molecules at liquid-liquid interfaces, which show the correct qualitative behaviour with respect to orientation and position (cf. graphic: Acetic acid molecule at a water-1-octanol interface).



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Transient Spectroscopy of Perovskite Solar Cells

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Transitent electrical measurements are widely used in the characterisation of perovsktie solar cells. A common method for the characterization of defects in conventional semiconductors is deep-level transient spectroscopy (DLTS). This technique is based on a modulation of the depletion layer, mostly by applying voltage pulses.

Due to the influence of field screening, redistribution of mobile ions and reduced conductivity of organic transport layers, charge carrier injection via voltage pulses depends often on man parameters including the temperature. This problem can be largely avoided by injecting via optical pulses, which enables us to record a rich trap spectrum over the whole temperature range down to 30K. We apply this technique, which is also known as photo induced transient spectroscpoy (PITS), to perovskites of various compositions and compare the results with complementary techniques. We show that multiple additional trap states can be observed when optical pulses instead of voltage pulses are used for injection. We use drift-diffusion simulations to visualize the cause of this behavior.

Doping of Organic Single Crystals for Thermoelectric Applications

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Doping of organic semiconductors boosts their technological potential for a wide range of thin film applications such as photovoltaics or lighting. In this contribution, we will address the implementation of doped molecular crystals in thermoelectrics (TE) which promise the recovery of substantial amounts of waste heat generated upon primary energy consumption [1]. For TE application it is desirable to use compounds with large Seebeck coefficient S, high electrical conductivity σ, and low thermal conductivity κ, which can be summarized in the dimensionless figure of merit at given temperature $zT = \frac{S^2\sigma T}{\kappa}$.

By methodically combining different acceptor and donor materials, the leading parameters of thermoelectric transport can be optimized selectively and even decoupled from each other. A concrete strategy to cope with this task enables the systematic modification of the band filling upon chemical doping of crystals composed of radical ions or polyaromatic hydrocarbons. The low thermal conductivity generic to van-der-Waals bound systems in combination with the superior charge mobility in single crystals offers an interesting approach towards organic thermoelectrics [2]. Moreover, electronic correlations in combination with the strong electron-phonon coupling in these materials can violate the Wiedemann-Franz law and, thus, lift the restriction of the interdependent optimization of electrical and thermal conductivity [3].

First results on the electrical and thermal properties of radical ion doped organic single crystals will be presented and evaluated regarding their thermoelectric potential.

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Time-dependent density-functional theory (TD-DFT) study on the donor-acceptor system WF3 / o-IDTBR

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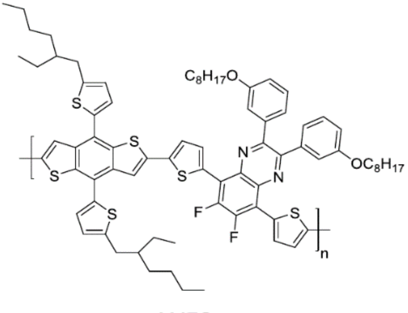
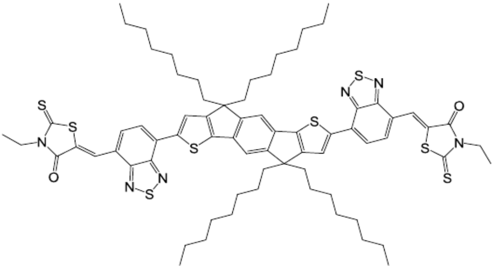
In recent years dono-acceptor systems with non-fullerene acceptors have attracted a lot of interest as active materials in photovoltaic applications. The electron donor-acceptor system WF3 / o-IDTBR, a non-fullerene acceptor photovoltaic blend, was studied with TD-DFT methods on the B3LYP/def2-TZVP level of theory. Calculated vertical excitation energies of both individual molecules and the interacting dimer agree well with experimental values. Local excitations and charge transfer excitations were identified by plotting difference densities between ground and excited state. TD-DFT was also able to provide an estimation of the energy barrier for the hole transfer from WF3 to o-IDTBR observed in transient absorption spectra



WF3



O-IDTBR

Photocatalytic Activity of Thickness-Controlled Bismuth Oxyhalide Nanoplatelets

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Abstract:

Many novel materials have been investigated for photocatalytic solar energy conversion leading to a comprehensive understanding of the underlying processes. [1] Layered bismuth oxyhalides (BiOX, X = F, Cl, Br and I) have recently drawn the attention of the field, because of their unique crystal structure which give rise to a highly active photocatalyst with extremely interesting and intriguing properties. These include e.g. complex interactions between Bi_2O_2 and halide layers, internal polarization and strong spin-orbit coupling analogous to lead halide perovskites. Dependent upon the exposed crystal facet, the internal field can be directed perpendicular or parallel to the flat surface, enabling control of the charge transfer direction. [2][3]

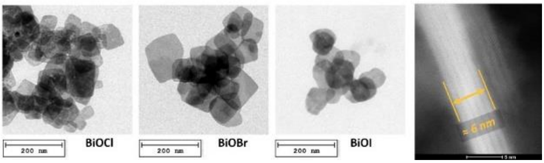

Figure 1: TEM images of thin BiOCl, BiOBr and BiOI nanoplatelets and HR-TEM image of a 6nm-thick BiOI nanoplatelet.

In this work we mainly study the influence of thickness on the photocatalytic activity and the internal charge carrier dynamics of bismuth oxyhalide nanoplatelets. The synthesized BiOX-nanoplatelets have thicknesses of several to tens of nanometers (see Figure 1) and lateral dimensions of 100 to 150 nm. We find high photocatalytic rates for H_2 evolution under UV and visible illumination as well as dependencies on thickness and on the concentration of oxygen vacancies. The apparent merits of efficient charge separation make BiOX nanocrystals highly promising also for overall water splitting.

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Structural composition of inverse opal structured $Ge_{1-x}Si_x$-Films and silylated $Ge_{9-x}Si_x$-ZINTL Clusters

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Routes to periodic porous materials of inorganic semiconductors are scarce. However, oxidative decomposition of ZINTL clusters in presence of a specific template leads to homogenous thin films. So far, we succeeded in preparing Ge films with inverse opal morphology and a well-defined pore size using solutions of the intermetallic compound K_4Ge_9 which contains nine-atomic clusters.[1] Herein we present studies of these Ge_xSi_{1-x}-films (x = 0, 0.25, 0.5, 0.75) revealing their elemental composition and oxidation states (XPS). Furthermore, we highlight carrier dynamics in these materials using Time Resolved Terahertz Spectroscopy (TRTS). We also show a reaction path for silylaton of these compounds and the resulting crystal structure. These silylated compounds are soluble in a broad variety of common laboratory solvents and therefore present an alternative approach to formation of porous films.

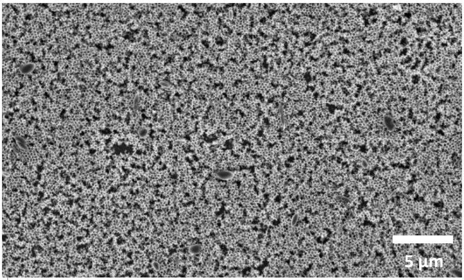

Figure 1. SEM picture of an inverse opal structured Ge_xSi_{1-x}-film (x = 0.75).

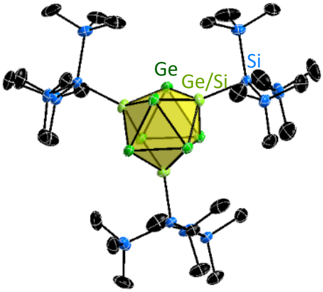

Figure 2. Silylated Si/Ge Cluster in [(K-2.2.2-crypt)($Si_{1.7}Ge_{7.3}(Si(TMS)_3)_3$].

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Supramolecular investigation of σ-hole electrostatic interactions

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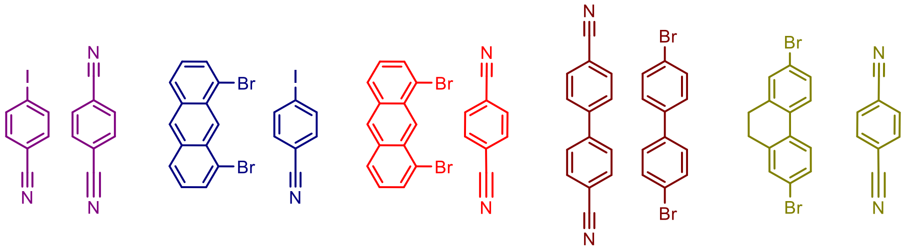
σ-hole exemplifies a region of positive molecular electrostatic potential (MEP) collinear with and opposite to covalent bonds to atoms of Groups IV–VII capable of forming highly directional electrostatic interactions with halogen bond acceptors.[1,2] The electron deficiency of the outermost lobe of the bonding orbital, hence the σ-hole, can be enhanced as the atom X becomes less electronegative and more polarizable (N < P < As < Sb, O < S < Se < Te and F < Cl < Br < I).[3] Depending on geometry and substituents of a molecule, positive MEP of sigma holes can be altered. The more electron attracting is the remainder of the molecule, the higher the positive MEP of the halogen atom. In this regard, we report our ongoing research on detection and quantification of receptor-substrate complexation relying solely on sigma hole electrostatic interactions by first performing deliberate synthesis of halogenated benzene, phenanthrene anthracene and pyromellitic dianhydride derivatives followed by supramolecular UV-Vis titration experiments and computational analyses.



Building blocks for highly directional σ-hole electrostatic interactions.

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Polymer-encapsulated Perovskite Nanocrystals: Synthesis and Optoelectronic Properties

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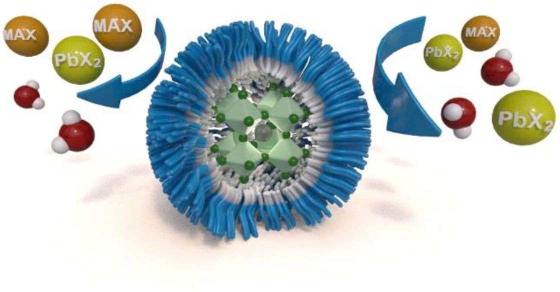
Halide perovskite nanocrystals (NCs) have shown impressive advances, exhibiting optical properties that outpace conventional semiconductor NCs, such as near-unity quantum yields and ultrafast radiative decay rates. Herein, we present a block copolymer-templated synthesis for perovskite NCs providing a drastically enhanced stability. [1] The polymer spontaneously forms micelles, which act both as nanoreactors and as a protective shell. Encapsulated by this polymer shell, the NCs display strong stability against water degradation and ion migration. Heterostructures of MAPI and MAPBr NC layers exhibiting efficient Förster resonance energy transfer (FRET), revealing a strategy for optoelectronic integration. Furthermore, we study the encapsulated NCs via single-particle spectroscopy and investigate the temperature dependence of the optoelectronic properties.



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Synthesis of Challenging o-Terphenyls via Domino Reactions: Entry to New Photoactive Materials

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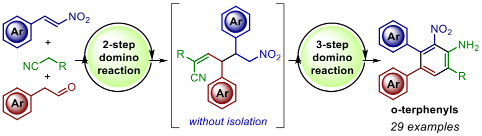
The domino process is a powerful tool to economically and sustainably build up complex molecular architectures.[1] The number of work-up and purification steps is drastically reduced, therefore, the multi-step procedure is less time-consuming and less waste producing, compared to the traditional stop-and-go synthesis.[1-4] Recently, we demonstrated a novel three-component two-step Knoevenagel/vinylogous Michael domino reaction starting from easily accessible arylacetaldehydes, malononitrile and nitroolefins towards *diaryl-substituted dicyanonitroolefins*, using imidazole as a cheap and commercially available organocatalyst.[5] Merging this two-step domino reaction with a facile $CuBr_2$/DABCO co-catalyzed three-step domino reaction in one-pot resulted in challenging *highly functionalized o-terphenyls*,[6] which are of potential importance for the synthesis of PHOLED-materials and therefore are of high interest for the development of new photoactive materials.[7] These recent results will be discussed in this presentation.



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Printed bulk heterojunction blends for photovoltaic applications

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The harvest of sunlight is a promising possibility to match the challenge of the continuously growing energy demand. Standard devices for light harvesting are commonly based on inorganic compounds. Over the last decades, photovoltaics based on organic components have emerged as an alternative to replace the conventional solar cells, due to their advantageous characteristics, such as light weight, flexibility, and solution processablity. Especially, since organic photovoltaics surpassed power conversion efficiencies of 11% [1], they have drawn attention in industry. The possibility to process this kind of solar cells out of solution enables the usage of low-cost manufacturing techniques, like roll-to-roll coating, spray casting or printing, which are large scale deposition methods and well established in industry.

Hence, taking the step towards large scale processing, the influence of these large scale methods on the performance of photovoltaic devices have to be studied. Since it is known, that the inner structure of the photoactive layer is an important key for an effective device, the influence of the printing process on the inner morphology of the photoactive thin film has to be investigated. Therefore, X-ray scattering techniques are suitable tools to probe the inside of these layers with the possibility to monitor the printing process in situ.

Therefore, we designed a meniscus guided slot-die printing set-up to perform in-situ X-ray scattering experiments on the evolution of the morphology of organic thin films during printing. This set-up was designed for grazing incidence small angle X-ray scattering (GISAXS) and grazing incidence wide angle X-ray scattering (GIWAXS).[2] Furthermore we investigated the morphological evolution of the donor-acceptor system PBDB-T:ITIC during the deposition process. This information is correlated to opto-electronic characteristics to get further insight in the relation between the inner morphology and the device performance. This correlation is needed to optimize the processing parameters to enhance power conversion efficiencies and the overall performance of organic solar cells.

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2D Materials and van der Waals Heterostructures for Applications in Photochemical Energy Conversion

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Two dimensional (2D) materials possess unique physical and chemical properties that make them promising candidates as high-performance compounds for future applications such as the renewable generation of fuels from sunlight [1]. Due to an extreme surface to volume ratio in 2D materials including highly catalytic defect and edge sites, optical excitations can couple to interfacial catalytic processes. Especially monolayer transition metal dichalcogenides (TMDs) in the form of MX2 with M being the transition metal (Mo, W) and X being the chalcogenide (S, Se) are of interest. They exhibit a suitable bandgap for light harvesting and large exciton binding energies [2] [3]. In this contribution, we successfully grew 2D MoS2 flakes on a Si/SiO2 substrate in the dimensions of tens of micrometers using chemical vapor deposition (CVD). Compared to mechanically exfoliated monolayers, these materials exhibit high photoluminescence intensities and narrow emission lines. Building on this synthesis procedure, we aim to grow both van der Waals and lateral heterostructures. Obtaining photo charge carriers in the form of interlayer excitons, the separated nanoscale charges from heterointerface edges can be used in photocatalytic systems. Therefore, these 2D heterostructures will be integrated into photoelectrochemical cells and configured as gate tunable working electrodes in a four terminal field effect transistor (FET) configuration. The goal of this work is to control energy band positions and carrier concentrations by gating the 2D heterostructure. Thus, we investigate coupled charge injection and chemical mechanisms at the solid 2D heterostructure/ liquid interface. Ultimately, we aim to realize selective (photo)electrochemical reactions by directing charge carriers to engineered catalytic sites by affecting catalytic overpotentials.

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Carbon-rich π-extended Helicenes

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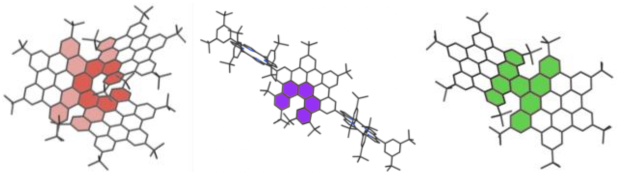
Over the past years, polycyclic aromatic hydrocarbons (PAHs) have gained of importance in the field of molecular materials, allowing us to understand in great detail the characteristics of planar PAHs. [1] The most exploited representative of the nitrogen-containing macrocycles – the porphyrin – shows different, but equally interesting properties. [2] Considering the unique features of the *i.e.* planar Hexa-*peri*-hexabenzoeconorone (HBC), non-planar helicenes and porphyrins have on their own, combination of at least two of these characteristics is expected to create much needed synergies in the field of molecular materials. Incentives for target molecules **1**, **2** and **3** are implementations into opto-electronic devices that are based on light harvesting, charge transfer, etc.



1 **2** **3**

Figure 1: Target molecules **1**, **2** and **3** (semi empiric PM6 calculated structures).

Molecules **2** and **3** have been successfully synthesized and characterized by standard analytical methods, showing unique fluorescent behavior.

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Tracking the impact of ternary sensitization on the performance and stability of organic solar cells

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Ternary sensitization of binary donor:acceptor blends has been demonstrated to be a promising way for enhancing the efficiency of organic solar cells [1,2]. This can be attributed to different beneficial effects of the third component in the absorbing layer, for example extending the absorption range or improving the morphology of the bulk heterojunction. Lately, ternary sensitization further was found to be a possible pathway towards increased long-term stability of organic solar cells [3,4]. By adding a third component, the morphology of the absorbing layer, which is essential for the device performance, can be stabilized against deteriorating influences of time and temperature.

In this work, six different fullerene derivatives are used to sensitize the absorbing layer of organic solar cells in order to investigate their influence on performance and long-term stability. For all ternary systems, the composition with the best power conversion efficiency is determined and the electrooptical properties are analyzed.

Furthermore, by storing devices at elevated temperature, changes in performance over time are tracked and the impact of the sensitizer on device stability in terms of electronic properties and morphology is analyzed.

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What is the initial stage of degradation mechanism for perovskite solar cells?

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Mixed organic-inorganic hybrid perovskite solar cells have shown a promising future because of their outstanding photoelectric performance. Solution processing makes it possible to achieve low-cost manufacturing of these solar cells. The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached the champion value of 24.2 % [1], making this technique competitive with commercial silicon solar cells. Despite all these advantages, the application of PSCs is currently limited by combining high performance and operational stability because PCE of PSCs can degrade due to presence of temperature, light, humidity and oxygen [2]. In addition, the rapid developing progress in the fabrication of PSCs has not accompanied the development of start-of-the-art characterization methods. Current degradation researche on PSCs is performed by simple current-voltage measurements. Therefore, it is necessary to introduce new characterization tools for analyzing the degradation mechanisms of PSCs. We investigated intial-stage degradation processes of different device architectures of PSCs under illumination conditions with in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small angel X-ray scattering (GISAXS) [3]. With this approach, we are able to follow the evolution of characteristic structures and of the inner morphology under illumination. After understanding the degradation mechanisms for different device architectures, potential solutions could be found to suppress the degradation.

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Advances in the growth of crystalline organic thin film

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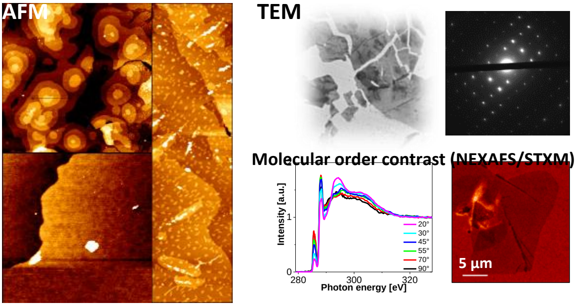
State-of-the-art organic semiconducting layers offer numerous advantages compared to conventional inorganic circuitry such as flexibility and low-cost processability. Still, numerous functional devices incorporating vacuum-processed films suffer from diffusion-limited growth leading to polycrystalline films reducing the efficiency of charge transport between electrodes. We explored advanced preparation techniques utilizing both the solid/liquid and various liquid/liquid interfaces as substrates.[1,2] Thin-film growth out of solution results in long-range ordered crystalline structures for a variety of both p- and n-type small molecules and is ultimately capable of overcoming common domain sizes and grain boundaries present in vacuum-deposited films. Our findings are supported by microscopic (AFM, TEM), diffraction (SAED) and spectroscopic (Angle-resolved NEXAFS, STXM) techniques as well as by charge-transport measurement data that excel reference data by one order in magnitude.



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Time-resolved scattering measurements to resolve perovskite formation

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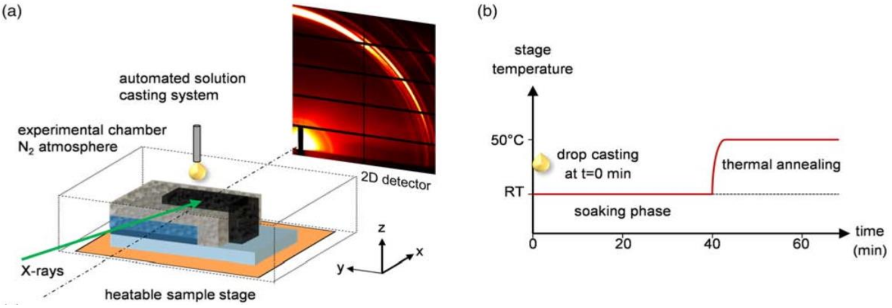
X-ray scattering can be used to resolve formation processes on the nanoscale within the dried film but also already during the drying of a thin film. This way it is possible, for example, to examine the influence of an additive on the structure formation process. Additives are frequently used to enhance material properties. For example, the addition of the processing additive 5-aminovaleric acid iodide (5-AVAI) applied to printed mesoscopic perovskite solar cells has a strong impact on the device performance and stability. However, the final nanomorphology does not differ significantly. The significant influence becomes apparent when the structure formation is examined in a time resolved manner. [1] We present our results and conclusions on this material system and discuss the possibilities for time-resolved scattering experiments.



a) Sketch of experimental set-up for time-resolved X-ray scattering experiments. b) External parameter changes during drying of film while measurements are taken.

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Tayloring the absorption in oxygen vacancy rich TiO_{2-x}-nanoresonators with anapole modes for enhanced photocatalysis in the visible

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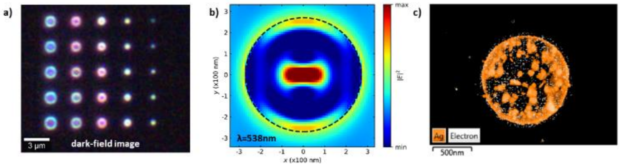
TiO_2 has been shown to be a good candidate as photocatalyst due to its excellent water adsorption properties, native surface catalytic activity and large band gap, thereby allowing for water splitting [1]. Thermal treatment of TiO_2 induces the formation of sub-bandgap oxygen vacancies states (OV-TiO_{2-x}) extending the material absorption from the UV to the visible spectrum [2]. In this work we shape OV-TiO_{2-x} into nano-disks (Fig. a) exhibiting anapole resonances [3,4]. This mode is characterized by the annihilation of its far-field scattering due to destructive electric and toroidal dipole interference, providing a maximum of electric energy inside the resonator (Fig. b). We show that by varying the nano-disk geometry we can spectrally locate the anapole resonance within the oxygen vacancy states and therefore boost the absorption of the particles. The absorption enhancement is monitored by the photocatalytic activity of the material under visible light illumination. As a proof of concept we demonstrate the exploitation of anapole modes by the preferred reduction of Ag on the surface of resonant disks under 532nm laser excitation at a single particle level (Fig.c). We further evince to which extend the anapole-driven absorption enhancement can be transferred to other materials with photocatalytic potential.



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Charge Recombination Dynamics in Defect-Engineered Organic-Inorganic Halide Perovskites

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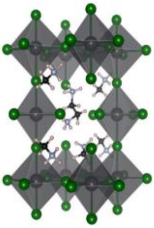
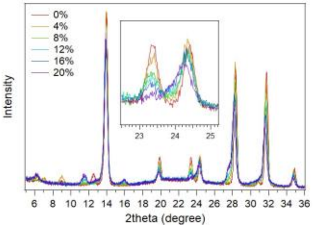
Organic-inorganic halide perovskites, with their ease of fabrication and bandgap-tunability, provide promising prospects in photovoltaic and light-emitting diode applications. While such materials are highly tolerant of defects, the presence of ionic, along with electronic, charge conduction can result in dynamic optoelectronic properties. In this work, we aim at understanding the charge recombination pathways in defect-engineered perovskites. Point defects are intentionally and controllably introduced into the lattice of methylammonium lead iodide ($MAPbI_3$), and the corresponding impacts to optoelectronic properties are systematically investigated. By manipulating the lattice strain, a series of thin films with tunable bandgaps from 1.60 – 1.71 eV are fabricated. In addition to the concentrations and energetic positions of defects, which are quantified by photothermal deflection spectroscopy, the effects of these defects on photoluminescence yield are studied by steady-state and time-resolved fluorescence techniques. This work not only sheds light on the interactions between organics cations and the inorganic lattice, the results also provide insights into the factors that underlie defect tolerance in hybrid halide perovskite semiconductors.





Tracking the morphology formation of printed non-fullerene active layers for solar cells by using GISAXS technique

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Non-fullerene organic solar cells (OSCs) have attracted great interests due to the low-cost materials and the highly tunable molecular energy levels. [1] The performance of OSCs is strongly influenced by the morphology of the active layer. Therefore, to understand the inner structure as well as the structure forming process of the active layer during drying kinetics is important for the device optimization in the future. [2]

In the present work, we fabricated an active layer which contains a low bandgap donor polymer (pffBT4T-2OD) with a non-fullerene acceptor (EH-IDTBR) for solar cells via slot-die printing technique. To observe the structure formation of the polymer domains, grazing-incidence small-angle X-ray scattering (GISAXS) was used during the printing process (Figure 1). In addition, atomic force microscopy (AFM) and scanning electron microscope (SEM) techniques were used to get the surface morphology information of the printed active layers.

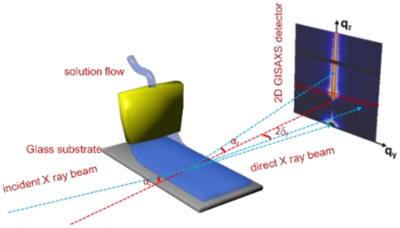

Figure.1 Schematic drawing of the simulation conditions of in-situ printing experiment process.

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Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks

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The potential of covalent organic frameworks (COFs) for realizing porous, crystalline networks with tailored combinations of functional building blocks has attracted considerable scientific interest in the fields of gas storage, photocatalysis, and optoelectronics. Porphyrins are widely studied in biology and chemistry and constitute promising building blocks in the field of electroactive materials, but they reveal challenges regarding crystalline packing when introduced into COF structures due to their nonplanar configuration and strong electrostatic interactions between the heterocyclic porphyrin centers. A series of porphyrin-containing imine-linked COFs with linear bridges derived from terephthalaldehyde, 2,5-dimethoxybenzene-1,4-dicarboxaldehyde and 4,4′-biphenyldicarboxaldehyde and thieno[3,2-*b*]thiophene-2,5-dicarboxaldehyde, was synthesized, and their structural and optical properties were examined. By combining X-ray diffraction analysis with density-functional theory (DFT) calculations on multiple length scales, we were able to elucidate the crystal structure of the newly synthesized porphyrin-based COF comprising thieno[3,2-*b*]thiophene-2,5-dicarboxaldehyde as linear bridge.[1]

Upon COF crystallization, the porphyrin nodes lose their 4-fold rotational symmetry, leading to the formation of extended slipped J-aggregate stacks. Steady-state and time-resolved optical spectroscopy techniques confirm the realization of the first porphyrin J-aggregates on a > 50 nm length scale with strongly red-shifted Q-bands and increased absorption strength. Using the COF as a structural template, we were able to force the porphyrins into a covalently embedded J-aggregate arrangement. This approach could be transferred to other chromophores; hence, these COFs are promising model systems for applications in photocatalysis and solar light harvesting, as well as for potential applications in medicine and biology.

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Rhenium and Manganese Complexes for Electrochemical CO_2 Reduction

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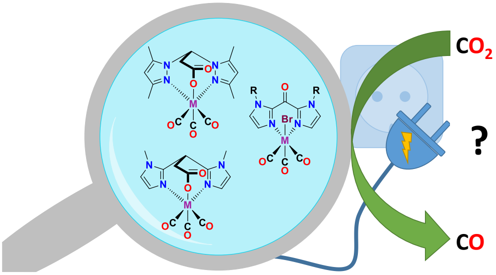
The conversion of CO_2 and thereby the reduction of the greenhouse gas is one of the major concerns of our society. Using CO_2 as a C1-building block to obtain value added products is highly desirable. Among others the solar energy driven electrochemical reduction of CO_2 is a very promising approach to reach those aims.[1] Metal complexes capable of CO_2 reduction are already well known since the 1980's. One of the first examples was a rhenium carbonyl complex [Re(bipy)$(CO)_3$Cl] published by Lehn *et al.*[2] This complex and several derivatives, as well as their corresponding manganese compounds have been thoroughly studied.

The common structural motif of these group 7 molecular CO_2 reduction catalysts is the facial carbonyl triad, one halogenido and a redox non-innocent *N*,*N*-donor ligand. In our group we alreay had complexes with a similar coordination pattern in hand.[3] The rhenium and manganese carbonyl complexes bearing either a bis(imidazolyl)- or bis(pyrazolyl)propionic acid ligands were investigated for their electrochemical properties under N_2 and CO_2 atmosphere. Furthermore, we designed novel rhenium and manganese complexes with bis(imidazolyl)ketone ligands. In contrast to the propionic acid-based ligands these chelating ligands provide a fully conjugated π-system which renders them superior to our priorly investigated scorpionate ligands. Our future aim is to enlarge the library of rhenium and manganese complexes by varying the bis(imidazolyl)-based ligand system.



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Selectively grown GaN Nanowalls for Photocatalysis: Growth and optical Properties

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GaN nanowires have gained increasing interest for photocatalytic applications due to their large surface-to-volume ratio and their excellent crystal quality. However, recent work has shown that NW sidewalls suffer from corrosion under illumination in water. [1]

As an alternative approach [2], we report the selective area growth of GaN nanowall arrays with different widths, orientations and distances on c-plane sapphire by molecular beam epitaxy.[3] Due to the special epitaxial relationship between sapphire and GaN [4], we achieved a precise control of the crystallographic plane of the nanowall-sidewalls. A dependence of nanowall width and the near-band edge photoluminescence on the crystal orientation of the sidewalls is observed and attributed to differences in the number of Ga dangling bonds in the respective plane. The transmission properties of nanowall arrays are investigated via experiment and simulation. We find a dependence of the distribution of the electric field on the nanowall dimensions which allows a precise tuning of the position of maximum field density.

Further, the high epitaxial control achieved by selective area growth enables the fabrication of more advanced structures like nano-grids or nano-scripts (see Supp. Info.). With these structures, an enhancement of the effective surface area by a factor of about five may be achieved, paving the way towards the efficient application in, e.g., nanofluidics or photocatalysis.

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Photoinduced electron transfer in supramolecular zinc phthalocyanine-fullerene hybrids

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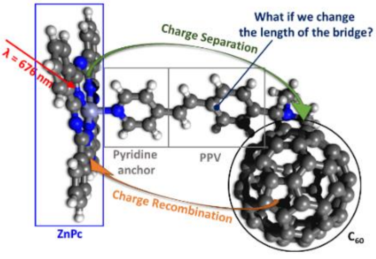
The investigation of photoinduced electron transfer in model systems is crucial for the understanding of electron transfer in biological systems. Zinc phthalocyanine as an electron donor protrudes due to its high extinction coefficient in the red region of the visible light, where the solar flux is at its maximum. In combination with C_{60} fullerene, an outstanding electron acceptor with extraordinarily low reorganization energy, we report photoinduced electron transfer in three supramolecular complexes. These hybrids differ in the length of the oligo-p-phenylenevinylene bridge (0, 1 or 3 units) and are connected by a pyridyl anchor for axial coordination to the zinc phthalocyanine. While no ground state interaction is observed, fluorescence quenching of zinc phthalocyanine centered fluorescence suggests strong excited state interactions. A variety of femtosecond and nanosecond transient absorption spectroscopy assays reveal fast electron transfer with the formation of the radical ion pair $\mathrm{ZnPc}^{\bullet+}$-$\mathrm{C}_{60}^{\bullet-}$ and slow charge recombination. A more profound examination of the kinetics in the context of Marcus theory locates the charge separation to the top and the charge recombination to the inverted region. Furthermore the electronic coupling decreases with increasing electron donor acceptor systems, while the reorganization energy increased. These trends are in stark contrast to findings in zinc porphyrin hybrids and the same electron acceptors.[1].



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Finding the right building blocks for molecular optimization - Mining a database of organic semiconductors

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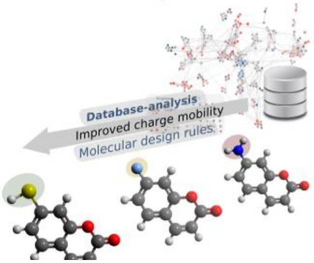
Abstract: Improving charge carrier mobilities of organic semiconductors is usually tackled by empirical structural tuning of a few promising compounds. Knowledge-based methods can greatly accelerate such local exploration by providing an overview of the problem-specific design space. Here, we provide an overview for organic semiconductors, from an in-house database of >64.000 organic molecular crystals, annotated with charge-transport descriptors that are calculated from first principles. This screening recovers many known and well-performing materials, while also uncovering many more promising candidates, not yet considered for organic electronics applications. Analysing the design space regions in this dataset by a chemical space network hints at already explored or promising regions. We further derive general design principles by evaluating the performance of molecular scaffold and sidegroup clusters of compounds. For these, we find certain scaffolds (sidegroups) to consistently improve charge-transport properties and uncover potential for improvement by functional groups, highlighting the usefulness of data-based approaches for a targeted design of organic electronics materials.



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Photochemical stability and photocarrier transport in $BiVO_4$ photoanodes for solar water splitting

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Bismuth vanadate ($BiVO_4$) has been actively investigated for hydrogen generation by solar water splitting because it absorbs visible light and, thus, allows efficient harvesting of the sun spectrum. It is one of the highest performance oxide photoanodes and possesses a theoretical solar to hydrogen efficiency of up to 9.2% [1]. Despite these advantages, $BiVO_4$ can suffer from photoelectrochemical (PEC) degradation [2] and is characterized by polaronic transport that can limit energy conversion efficiencies. In the first part of our work, we investigate the contributions of electronic and chemical processes that are responsible for the temporally decreasing photocurrent under operating conditions using PEC experiments. Using X-ray photoelectron spectroscopy, we further analyze how chemical modifications of the $BiVO_4$ surface affect charge trapping and photocatalysis at the semiconductor/liquid interface. In addition to surface instabilities, the PEC performance of $BiVO_4$ is limited by low charge carrier mobilities caused by the formation of small-polarons and carrier trapping by defect states [3]. Therefore, the second aim of our research is to provide improved understanding of small-polaron transport and native defect energetics within $BiVO_4$. Since polaron hopping is a thermally activated process, we perform temperature-dependent conductivity measurements to determine the hopping activation energy. Furthermore, it is not yet fully understood how polarons interact with different defects. Hence, we intentionally alter the type and density of defects and analyze the role of defects and polarons on the charge transport. Together, improved understanding of coupled physical and chemical processes at the surface and in the bulk will allow improved performance of $BiVO_4$ and inform efforts to develop new metal oxide photoelectrodes.

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Dimensional reduction of halide double perovskites: Insights from first principles calculations

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Dimensional reduction of the inorganic sublattice of organic-inorganic (hybrid) halide perovskites ABX_3 can be used to achieve electronic confinement in bulk solids, without the need for nanostructuring. Quasi-2D perovskites feature metal-halide sheets with *n* layers of an ordered perovskite lattice, separated by organic cations. Lead-based quasi-2D halide perovskites [1] exhibit larger band gaps, less disperse bands and higher exciton binding energies than their 3D counterparts [2]. Double perovskites, a generalization of ABX_3 with two different B site cations, exhibit an even wider array of compositions and electronic structures, with band gaps between about 1 eV and 3.5 eV depending on composition [3]. Quasi-2D derivatives of the double perovskite $Cs_2AgBiBr_6$, corresponding to structures with one and two layers of alternating $AgBr_6$ and $BiBr_6$ octahedra, have recently been reported [4].
Here we present first principles calculations of quasi-2D double perovskite derivatives with *n*=1-4 using density functional theory and Green's function-based many-body perturbation theory. For AgBi-based systems, our calculations reveal a conversion from an indirect to a direct band gap, as the inorganic lattice is thinned to a monolayer. We separate the effects of reduced dimensionality from those of structural distortions and strong spin-orbit coupling. Our results suggest optoelectronic properties distinctly different from typical quasi-2D lead-halide perovskites.

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Machine-Learned Chemisorption Model for CO_2 Electroreduction on Carbide Catalysts

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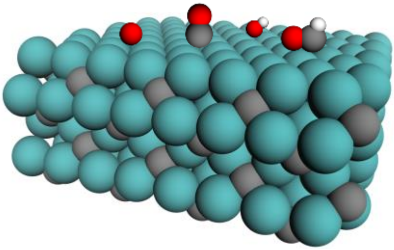
A drastic reduction of CO_2 is urgently needed to fight climate change and enable a sustainable growth. The electrochemical reduction of CO_2 (CO2RR) is a promising approach to generate chemical energy carriers from renewable electricity. In order to meet global demand, CO2RR would ideally be catalysed by non-noble metals [1]. In this respect, transition metal carbides (TMCs) are a promising material class, with e.g. Mo_2C recently reported to convert CO_2 into CH_4 at low potentials of ~0.55 V [2]. Considering the wide variety of structural and compositional motifs exhibited by TMC surfaces, this finding is possibly only the top of the iceberg though and even better CO2RR TMC catalysts might exist.



In order to efficiently explore this wide chemical space and the concomitant potential of TMCs for CO2RR, we therefore establish a machine learning model from first-principles data to predict the adsorption energies of important surface species for CO2RR including *CO, *CHO, *O and *OH for a variety of TMC surfaces and compositions. These energies reveal a profound break of scaling relations that were previously established for transition metal (TM) and TM oxide catalysts and that limit the CO2RR performance for these materials classes [3,4]. This break of scaling relations can be rationalized by the simultaneous presence of metal and carbon active sites at the surface of TMC catalysts.

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Magnetic Nanoparticles as Catalyst for Molecular Solar Thermal (MOST) Energy Storage and Release Systems

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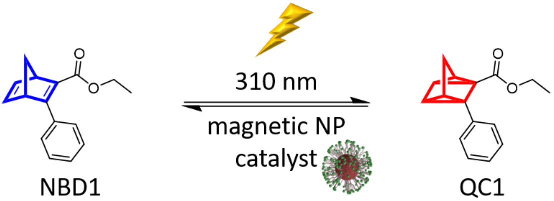
Molecular solar thermal (MOST) energy storage and release systems are a promising supllement to common photovoltaics. Within these systems the solar energy is harvested and stored on a molecular level; when needed it can be released as thermal energy.[1] One of the most prominent examples of MOST systems is the interconversion of norbornadiene (NBD) and quadricyclane (QC).[2] Herein we present an efficient and elegant way to release the energy, which is stored in the strained carbon scaffold of the metastable QC. By anchoring a Co(II)-Salphen complex onto Fe_3O_4 nanoparticles, we obtained the magnetic catalyst [Fe_3O_4-CoSalphen]. This quasi-homogeneous catalyst based on magnetic core-shell nanoparticles shows excellent activity in combination with good durability. Furthermore, tedious purification steps are rendered unnecessary, since the catalyst can simply be removed by the action of an external magnet. Our magnetic catalyst [Fe_3O_4-CoSalphen] in combination with the readily available interconversion couple NBD1/QC1 (Scheme 1) shows great potential for technical applications as MOST energy storage system.[3]



Scheme 1: *The interconversion couple NBD1/QC1, photoisomerization to the metastable energyrich QC1 is achieved by irradiation with 310 nm light. The stored energy can be released catalytically with the novel magnetic catalyst [Fe_3O_4-CoSalphen].*

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Hierarchically Structured DSSCs Mediated by Hydrogen Bonding

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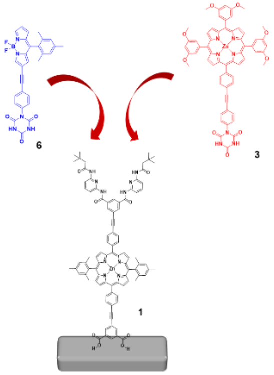
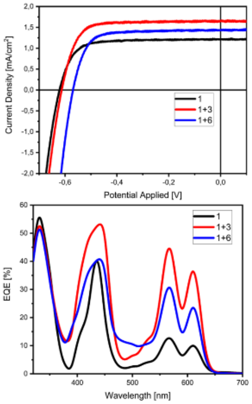
The controlled self-assembly of functional molecules on surfaces is of paramount importance for the fabrication of devices.[1] Next to the attachment of covalently anchored self-assembled monolayers (SAMs), also the implementation of non-covalent forces like hydrogen bonding is an excellent tool towards the formation of highly ordered superstructures.[2] We report on a unique approach combining the covalent surface attachment of organic dyes, equipped with either Hamilton receptor or cyanuric acid moieties, together with the advantages of a highly directional non-covalent postfunctionalization mediated by hydrogen bonding. The resulting photoactive nanohybrids were successfully implemented in dye sensitized solar cells to yield a significant increase in the overall efficiency, due to the non-covalently added 2nd dye layer.





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Oriented Thin Films of Electroactive Triphenylene Catecholate-Based Two-Dimensional Metal–Organic Frameworks

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Two-dimensional metal-organic frameworks (2D MOFs) are crystalline and porous materials consisting of rigid organic building blocks that are interconnected through square-planar coordinating metal-ions, forming 2D extended sheets. The self-organization of these sheets yields a highly ordered layered material featuring defined pore sizes and shapes. The combination of the well-defined molecular stacks with electrical conductivity renders 2D MOFs intriguing candidates for optoelectronic applications.[1] The incorporation of this class of materials into diverse types of devices requires the growth of 2D MOFs as thin films on different substrates.[2] Control over the growth process with regards to the film coverage, thickness, roughness and crystal orientation is of paramount importance for the realization of future MOF-based functional devices.

Herein, we present the synthesis of the electroactive metal-catecholate (M-CAT) series as oriented thin films by vapor-assisted conversion (VAC).[3] The M-CATs comprise the conjugated tricatecholate, 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP), and square-planar coordinated metal ions such as Ni(II), Co(II) and Cu(II).[4-5] Crystalline and oriented thin films were grown on gold substrates featuring high surface coverage. The use of a modulator in the synthesis protocol enabled the successful growth of high-quality oriented M-CAT films on glass, quartz and ITO substrates. Electrical conductivity measurements of the M-CAT films revealed high values in the range of 10^{-3} S cm^{-1}. Highly-defined M-CAT films on quartz substrates enabled their advanced photophysical characterization by means of UV-Vis, photoluminescence (PL) and transient absorption spectroscopy.

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Tuning Selectivity of Electrochemical CO_2 Reduction and Hydrogen Evolution Reaction on Metal Modified Si/SiO_2 Electrodes via Bicatalytic Mechanisms

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The efficient conversion of the greenhouse gas CO_2 to fuels with sunlight is a milestone for sustainable energy economy. An appropriate catalyst for the CO_2 reduction reaction must be stable, selective towards the desired product, and has to lower the kinetic barrier significantly. We present two types of mesoscopic structured metal based electrodes exhibiting a change in activity and selectivity for hydrogen evolution reaction (HER) and CO_2 reduction reaction (CRR). These changes are attributed to two different bicatalytic mechanisms:

The structuring of silicon based photoelectrodes with gold discs, which are fabricated by lift-off nanoimprint lithography [1], shows an enhanced HER reactivity, depending on the geometric properties of the gold discs [2]. The results indicate a bicatalytic mechanism taking place at the metal/oxide phase boundary.

In our second approach we aim to take advantage of a metal/metal bicatalytic effect found by the group of Jaramillo. The authors showed an enhancement of the selectivity of CRR on electrodes consisting of gold nanoparticles on copper towards products containing C-C bonds such as ethylene at low overpotentials [3]. They suggest complementary chemical reactions taking place on both metals in close proximity leading to a tandem mechanism [3]. We present an inter-digital-array electrode configuration, where we are able to address the two metals individually. This allows for optimization of the potential dependent product distribution while further investigating the involved bicatalytic mechanism.

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Tracking nanobubble generation with iSCAT

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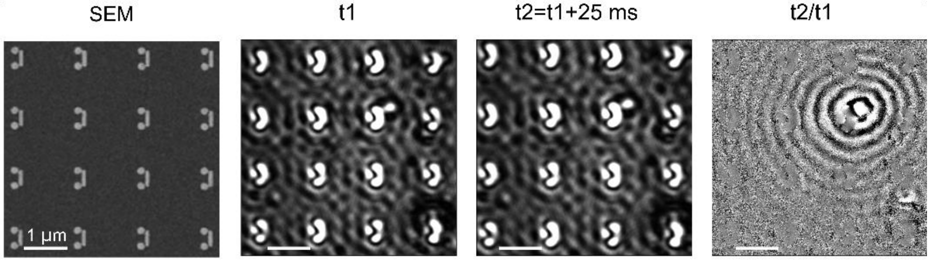
Plasmonic-assisted photocatalysis has attracted considerable interest due to the possibility of tuning the absorption frequency of metallic antennas over the solar spectrum, providing more flexibility compared to semiconductor photocatalysis. A number of reactions with great technological interest for energy storage and conversion are gas-generating. Gas production in the form of nanobubbles (NBs) at the single particle level is particularly difficult to detect *is-situ* with optical techniques, due the small size and low scattering cross-section of NBs. Up until now, NBs generation has been mainly investigated by dark-field [1] or fluorescence microscopy [2].
In this context, we apply label-free interferometric scattering microscopy (iSCAT) [3] to further improve the sensitivity and time resolution of NBs detection. The interferometric detection allows the identification of objects much smaller than what is achievable with dark-field microscopy. At the same time, the scattering signal is not affected by saturation or blinking effects, which impose a limitation on laser power and achievable imaging speed in fluorescence microscopy. We monitor with iSCAT ethanol reduction induced by illumination with an 808 nm laser on resonant gold antennas. In order to highlight the generation of NBs we employ differential imaging, suppressing all static features. Nanometer localization of the NBs growth can also be achieved by 2D Gaussian fitting of the NBs point-spread function.



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New Soluble Precursors for Porous Thin Films and their Behavior in Solution

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A wet-chemical synthetic route from soluble Ge_9 clusters to inverse opal thin films of elemental germanium was recently established.[1] This preparative process could be successfully transferred to other tetrel elements, like Si, mixed Si/Ge or Sn – aiming for applications in energy conversion and storage.[1, 2] Beside the soluble tetrel compounds A_4E_9 (A = alkali metal; E = Ge – Pb) and $A_{12}E_{17}$ (A = alkali metal; E = Si – Pb) with a versatile and relatively well understood reactivity, we aim for new element combinations, applicable for the preparation of thin films to allow for the tuning of their properties. For this reason, we expand our research on further soluble element combinations, as bimetallic systems Ge/P or Sn/Bi or trimetallic Sn/Ge/Bi. First steps in this region are already undertaken and metallic Sn-Bi-thin films from soluble K_2SnBi are obtained. To enhance our knowledge, we also investigate the behavior of these systems in solution and present first results of formed soluble species.

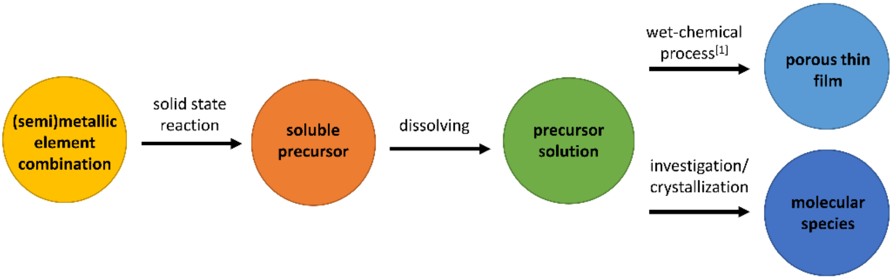

Figure 1: General pathway for the synthesis of soluble (semi)metallic precursors for the preparation of porous thin films or as molecular species for reactions in solution.

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Impact of bridging ligand substituents on photocatalytic water oxidation by supramolecular ruthenium macrocycles

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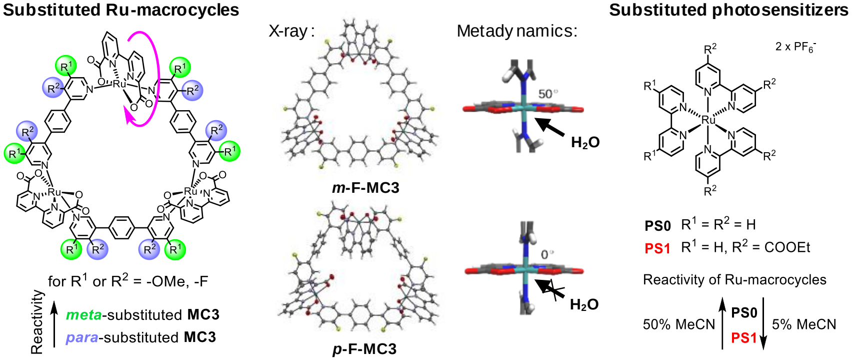
The light-induced splitting of water into its elements has attracted particular attention as a sustainable energy source. [1] Recently, we have reported that macrocyclic Ru-complex **MC3** exhibits high catalytic activity for chemical water oxidation under acidic conditions. [2, 3] Here we present a series of **MC3** derivatives that contain different substituents in the bridging ligand. Their photocatalytic activities in water oxidation were studied using a three-component system based on a $[Ru(bpy)_3]^{2+}$ photosensitizer, a sacrificial electron acceptor and the supramolecular catalyst at a neutral pH. X-ray analysis and metadynamics simulations revealed that the catalytic activity of the macrocycles is considerably dependent on the regioisomeric position of the bridging ligand substituents. Furthermore, the use of ligand-substituted photosensitizers allowed us to identify solvent-dependent effects that have a substantial impact on photocatalysis.



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Copper(II) salts as viable dopants for organic semiconductor charge extraction layers in perovskite solar cells

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In n-i-p type conventional hybrid lead halide perovskite solar cells (PSC), the uncontrolled air-oxidation of spiro-OMeTAD hole transport layer (HTL) with copious amounts of redox-inactive, hygroscopic Li-TFSI and *tert*-butylpyridine (t-BP) additives is shown as one of the main reasons for poor reproducibility and stability of the devices. [1] Despite a few direct p-dopants are reported for spiro-OMeTAD HTL, the maximum device performance is achieved only with high dopant concentrations and Li-TFSI/t-BP additives and thus, not resolving the stability and reproducibility issues. [2,3] Recently, we reported Li-TFSI and t-BP free, highly reproducible and stable planar PSCs with doped spiro-OMeTAD HTL containing small amounts (2-4 mol%) of a commercial Cu(II) salt, $Cu(TFSI)_2$, as p-dopant. The HTL was prepared by industrially relevant thermal co-evaporation technique. [4] This method opens the possibility of exploiting different combinations of dopants and organic semiconductors as HTL, which are not feasible through conventional solution processing technique.

In this line, here we report a study on a different Cu(II) salts as direct p-dopants for spiro-OMeTAD and N,N,N′,N′-Tetrakis(4-methoxyphenyl)benzidine (OMe-TPD) hole transport materials. The direct p-doping of spiro-OMeTAD and OMe-TPD is characterized by the UV-vis absorption, X-ray photoemission spectroscopy (XPS) and conductivity measurements in solution and in the solid state. The impact of Cu(II) salts counteranion on their redox properties and consequent changes in the valence band energetics of the doped HTL in the bulk and at the perovskite/HTL interface are studied in detail by using ultraviolet photoemission spectroscopy (UPS). Finally, PSCs are prepared with these Cu(II) salts doped HTLs and their impact on device performance is studied and compared.

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General strategy for tunable low-LUMO B-doped polycyclic aromatic hydrocarbons by electrophilic borylations

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Boron-doping is an efficient strategy to manipulate frontier molecular orbital energies of graphene or related polycyclic aromatic hydrocarbons (PAHs). Nevertheless, the use of boron-doped PAHs in electronic materials is still scarce. This is due to the fact that the empty p_z-orbitals of three-coordinate B-doped PAHs, which account for their excellent electron accepting properties, can reduce chemical stability and impede synthetic efforts. We have developed a new approach that enables the synthesis of doubly boron-doped PAHs from a great variety of simple alkene precursors via a metal free hydroboration/borylation cascade. [1] With this method a series of air-stable doubly boron doped analogues of pyrene, perylene and anthanthrene could be obtained. This allowed us to clarify the effect of shape, size and structure of boron-doped PAHs on optoelectronic properties. Further tuning of properties via post-synthetic functionalization afforded sublimable low-LUMO three-coordinate boron-substituted PAHs and led to the first implementation of such a molecule as an acceptor material in organic solar cells with power conversion efficiencies (PCEs) of up to 3 %. [2]

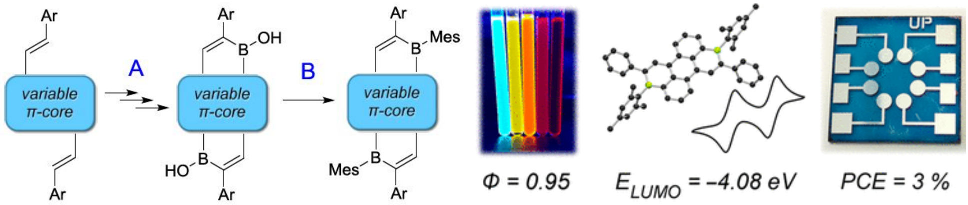

Figure 1: Reaction scheme (left) and outstanding properties (right) of the synthesized B-doped PAHs.

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Tuning the transition dipole moment of $CsPbBr_3$ nanoplatelets for improved light outcoupling of blue light-emitting diodes

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The unique optical properties of lead halide perovskites have drawn significant attention towards their application in light emitting devices (LEDs) in recent years. While quantum yield, emission wavelength and stability are already in the focus of many research groups, the orientation of the emissive transition dipoles has rarely been investigated. As known from other thin film applications, such as organic LEDs, this quantity can severely affect the light outcoupling of the device and thereby limit the external quantum efficiency.

In this work, we investigate $CsPbBr_3$ nanoplatelets (NPl) of variable thickness and determine the orientation of their transition dipole moments (TDM) from thin film radiation pattern analysis. We then apply optical simulations to elucidate the performance limits of perovskite based blue LEDs in prototypical device architectures. As was already shown, the TDM of $CsPbBr_3$ nanocrystals can be tuned from preferentially vertical in nanocubes to horizontal in ultra-thin NPls [1, 2]. At the same time, quantum confinement renders the emission color from green to deep blue. Here, we use a systematic thickness variation from 2 to 6 monolayer thick NPls to study the tunability of the TDM orientation and the concomitant color shift. We find that with increasingly beneficial horizontal orientation, the outcoupling efficiency increases to values close to 30 %. However, since the photoluminescence quantum efficiency degrades considerably for decreasing thickness [3], the overall maximum device efficiency does not significantly improve beyond 20%. Thus, for the currently available material sets we can conclude that while the non-ideal orientation limits device performance for nanocubes, devices with NPls are limited by non-optimal PLQYs. Nevertheless, our results reveal very promising new efficiency limits for solution-processed light emitting diodes.

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Tetrahydroxy-Perylene Bisimide Embedded in Zinc Oxide Thin Film as Electron Transporting Layer for Non-fullerene Organic Solar Cells

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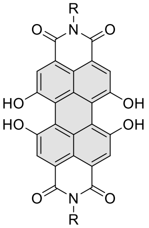
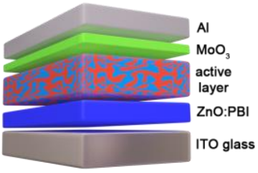
The last decade showed a growing diversity of perylene bisimide (PBI) materials for applications in organic field-effect transistors and organic solar cells (OSCs). PBIs owe their popularity to their outstanding optical properties, high charge carrier mobilities and stability.[1] The development in the fields of PBI-based transistors and OSCs went hand in hand with the progress in their synthetic methodology. Our recent synthetic protocol[2,3] gave access to tetra-hydroxy-bay-substituted PBIs offering coordination sites for metal ions. The new ligands were dispersed into zinc oxide (ZnO) films to fabricate organic-inorganic interlayers in which PBI acts as a photosensitizer of semiconductive ZnO thin films. In the poster, we will present a successful utilization of these hybrid materials as photoconductive cathode interlayers in the inverted OSCs. The presence of PBI molecules enhanced conductivity of ZnO leading to power conversion efficiencies of up to 15.95% for a non-fullerene based organic solar cell.[4]





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X-ray diffraction studies of lead halides perovskites, from nanoparticles to single crystals

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Lead halide perovskites (LHP) exhibit optoelectronical properties usually associated with highly ordered semiconductors. We employ x-ray and neutron techniques to probe the degree of structural order and disorder in LHP single crystals and nanoparticles. In the case of LHP nanoparticles (synthesized in the groups of A. Urban [1] and L. Polavarapu at LMU Physics) we probe nanoparticle sizes, crystallinity, and their arrangements in solution by a combination of small angle scattering and Debye Scherrer diffraction [1,2,3]. Furthermore, we develop high energy x-ray diffraction schemes [2] to quantify disorder in LHP single crystals. For this purpose we measure diffuse scattering at ambient and low temperatures. The diffuse scattering contains a contribution from phonon modes. The single crystals for these experiments are grown by Julian Höcker from ZAE Würzburg (V. Dyakonov, A. Baumann).

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Fundamental characterization of intramolecular singlet fission materials and mechanistic insights

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Studies concerning the efficiency of solar cells have been at the forefront of investigations in recent years. Strategies as to how to increase the overall efficiency have been elaborated for decades: One of them is the singlet fission (SF) process. In SF, one singlet excited state is converted into two triplet excited states. Such a conversion has the potential to overcome the Shockley-Queisser limit, namely around 30%, and to increase it up to approximately 45%. [1] Various molecular materials have emerged as potential candidates for undergoing SF. We, for example, focus on the photophysical characterization of SF and, therefore, on the understanding of all the intricacies of SF. This is done by means of steady-state absorption and fluorescence spectroscopies, which are complemented by time-resolved transient absorption spectroscopy, of novel SF materials. By utilizing carefully tailored spacers as a means to link, for example, two chromophores, we are able to probe the influences on the efficiency of the singlet to triplet excited state conversion and, in turn, to improve our overall understanding of SF.

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Colloidal Perovskite Nanocrystals: Shape-controlled Synthesis and Self-assembly

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Perovskite nanocrystals (NCs) are gaining increasing attention in many fields ranging from chemistry to physics and engineering owing to their extremely interesting properties such as high photoluminescence quantum yield (PLQY), tunable optical bandgap, enhanced stability, ease of preparation and solution processability. (1-3) In the poster, I will present solution phase synthesis of perovskite NCs (nanocubes, nanoplatelets, nanowires, and nanorods) with excellent monodisprsity, and bright photoluminescence (PL) extended across the entire visible spectral range. The morphology of perovskite NCs can be easily controlled from nanocubes to nanoplates (NPls) and nanowires (NWs) by means of simple chemistry such as precursor ratios and ligand concentration (1-3). Thus, the optical bandgap of the perovskite NCs is tunable by morphology as well as halide (Cl, Br, and I) composition. The PL efficiency of perovskite NCs can be hampered by surface defects, which can be repaired by post-synthetic surface treatment to achive nearly unity PLQY (4).

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Interface morphology of nanoscopic organic solar cells

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The orientation of organic semiconductors at the p/n junction interface plays an important role in the energy level alignment and the charge separation process of an organic solar cell. In typical bulk-heterojunction solar cells, the relative orientation of donor and acceptor directly at the interface is not controlled. We have developed a methodology to assemble nanoscale planar p/n junctions with deterministically controlled morphology. In our work, we discuss how nanofibers of the organic semiconductor P3HT with a defined molecular orientation can be used together with fullerenes to build a nanoscopic solar cell with a controlled interface morphology. Additionally, we have performed nanoscale electrical measurements for the electrical characterization of single component nanofibers. [1]

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Mechanically Interlocked Single-Walled Carbon Nanotubes

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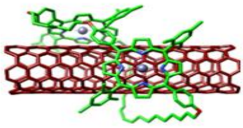
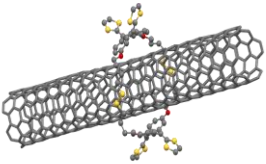
Herein, we report on the comparative study concerning mechanically interlocked SWCNTs (MINTs). On one hand, macrocyclic porphyrin rings were mechanically interlocked with SWCNT threads (MINT-porphyrin) and, on the other hand, the reversible formation and breakage of ex-TTF disulfide bonds were employed for the construction of macrocycles around SWCNTs (MINT-exTTF). The formation of MINTs was corroborated by means of electron microscopy. Moreover, their stability was investigated under a varity of experimental conditions. From a full-fledged characterization of the MINTs by means of UV-vis-NIR absorption, fluorescence, Raman, and transient absorption spectroscopy we demonstrated chiral selectivity / flexibilty in the overall MINT formation. The strongest fluorescence quenching in steady-state experiments is associated with the fastest excited state decay in time-resolved measurements.



MINT-porphyrin



MINT-exTTF

Of great importance is the fact that stronger electronic interactions were found between the electron donating porphyrins / ex-TTFs and smaller diameter SWCNTs when compared to their larger diameter analogous.

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Intrinsic Exciton Confinement in a *quasi*-0D Bismuth-based Alternative to Lead Halide Perovskites

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Lead halide perovskites possess highly interesting optoelectronic properties, but the toxic nature of the constituent lead drives the quest for more benign alternatives. Bismuth-based perovskites are of particular interest because of the isoelectronic structure of Bi^{3+} and Pb^{2+}. In this context, we report the preparation of hexagonal $Cs_3Bi_2I_9$ nanoplatelets with thickness of 8-10 nm and lateral sizes up to half a micrometer. We further apply a combination of first-principles density functional theory (DFT) and Green's function-based many-body perturbation theory calculations as well as time-integrated and time-resolved optical measurements to elucidate the unusual properties of this material and explain the reasons for its weak photoluminescence. Moreover, we identify a strong excitonic transition in the absorption spectrum and discuss the origin of its large exciton binding energy. The study demonstrates that bismuth-based perovskites offer unique optical and electronic properties promising for future applications in light harvesting devices.

Analyzing the pressure dependency of ruthenium-based PCET reagents

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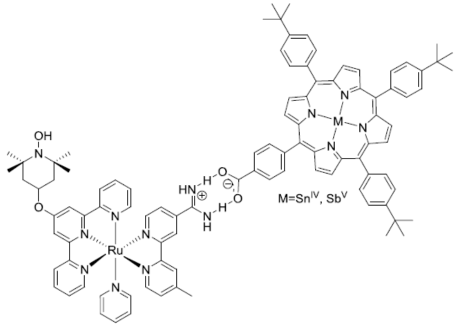
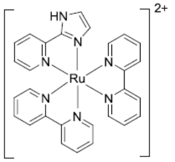
Thermal, electrochemical and photochemical proton-coupled electron transfer (PCET) governs the chemical energy conversion in natural and artificial systems. [1] Our approach of pressure and temperature dependent measurements by NMR spectroscopy or via stopped-flow and electrochemical [2] analysis will be applied for detailed clarifying of the variety of PCET mechanism such as bidirectional, unidirectional, inter- and/or intra-molecular as well as selfexchange PCET and HAT (hydrogen atom transfer) processes.

To that goal we synthesized specific ligands containing amidinium, TEMPO or imidazol residues and their ruthenium complexes that are predestinated for long-range PCET, HAT and self-exchange mechanisms.





Moreover, we will synthesize dinuclear ruthenium compounds for the investigation of multiple PCET reactions. High pressure techniques will allow us to analyse the kinetic and thermodynamic behavior of these reactions.

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Insights on photocatalytic hydrogen evolution with [FeFe]-hydrogenase mimic dyads

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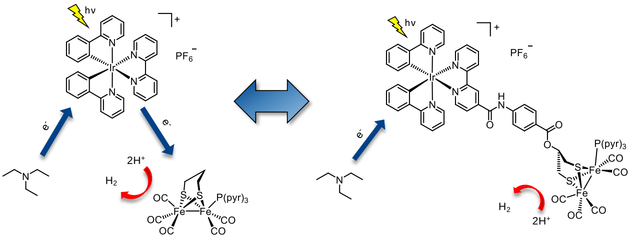
Because of the continual growth of worldwide energy demand and the global warming the interest in an eco-friendly energy carrier generation becomes more and more important. One possibility to achieve this goal is hydrogen evolution by photocatalytic water splitting. In our research we focus on [FeFe]-hydrogenase mimics as catalyst and use them in combination with transition metal organic complexes like Tris(bipyridine)ruthenium(II) chloride or Bis(2-phenylpyridine)(bipyridine)iridium hexafluorophosphate as photosensitizer. Beside these multi-component systems, we also synthesized photocatalytic dyads by linking a [FeFe] catalyst covalently to the different photosensitizer moieties and characterized their catalytic performance as well as their spectroscopic and electrochemical properties in comparison to the respective single-molecule system. To perform the photocatalysis in pure water, the water insoluble [FeFe]-catalyst is solubilized with poly(2-oxazoline) micelles.[1]



We could show that the single-molecule systems perform significant better compared to their corresponding dyads. We assume that this issue is elicited on the one hand by the distinct reductive quenching mechanism of the photocatalytic systems and on the other hand by the fostered charge recombination process in the dyad framework.

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Dye-Containing Covalent Organic Frameworks

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Due to their extended π-conjugated molecular scaffolds and visible light absorption abilities, semiconducting organic dye molecules have been widely incorporated in organic electronic and photovoltaic devices such as organic field effect transistors (OFETs) or organic solar cells (OSCs). Since their performances are strongly influenced by the molecular arrangement of the active components, the implementation of these chromophores as building blocks into crystalline, two-dimensional polymers, *e.g.,* covalent organic frameworks (COFs), [1] makes such materials promising candidates for electroactive materials. [2] Recently, we reported on the implementation of functionalized diketopyrrolopyrrole (DPP) derivatives as semiconducting subcomponents into crystalline 2D imine [3] and boronate ester [4] COFs. Enhanced light harvesting in the visible region was observed for both COFs and electrical conductivity measurements for a boronate ester COF revealed conductivity values of up to 10^{-6} S cm^{-6}. [4] To further enhance the scope of chromophore-containing COFs, we are also working on the incorporation of other dyes, *e.g.,* boron-dipyrromethenes (bodipy), in order to obtain functional materials with high light absorption ability and interesting optoelectronic properties.

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In-situ GISAXS/GIWAXS measurements on slot-die printed thin-film perovskite layers for solar cell application

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Thin-film organic-inorganic metal halide perovskite based solar cells (PSCs) are currently intensely researched for their potential as cheap, ultrathin and flexible next generation solar cells. Reaching minimodule efficiencies of around 17% in 2018 and 15% on ultrathin flexible substrates commerzialisation is promising. However, further improvement on upscaling is needed in order to push PSCs to the market. Especially the development of industrial compatible deposition methods without losing efficiency requires further research and development.[1] In principle, industrial requirements can be met by roll-to-roll slot-die coating.[2] Highly crystalline and uniform films with low defect concentrations are paramount in reaching high power conversion efficiencies in PSCs.[3] GISAXS and GISANS (grazing incidence small angle x-ray and neutron scattering) measurements are well suited to probe the influence of temperature, ambient moisture, printing parameters and precursor composition on crystallization kinetics and crystal film quality by probing stochastically relevant large sample areas.[4-5] I*n-situ* GISAXS and *in-situ* GIWAXS measurements were performed on methyl ammonium lead iodide (MAPI) thin films during slot-die printing. Drying and crystallization kinetics were investigated for different printing temperatures. In order to easily apply findings to solar cell fabrication prototypical MAPI was printed on a glass/ITO/PEDOT:PSS layer structure. Transient GIXS measurements are well suited to show kinetics during film drying and subsequent annealing steps and can be broadly applied to different perovskite materials, deposition methods and substrate materials.

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Superpyridine: An *N*-heterocyclic hexa-*peri*-hexabenzocoronene

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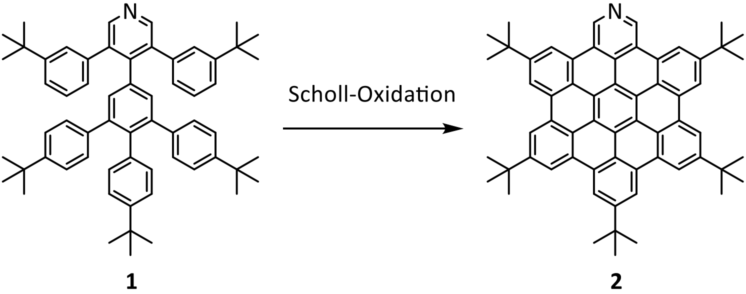
In the scope of polycyclic heteroaromatic compounds and heterocyclic nanographenes[1], we developed the first efficient synthesis for the *N*-heterocyclic hexa-*peri*-hexabenzocoronene **2** that may be called “superpyridine”. The key step was successful cyclodehydrogenation of precursor molecule **1**, in which all bonds connected to the pyridine ring are already existent. Target molecule **2** was characterized by NMR-spectroscopy in detail, mass spectrometry and UV-Vis spectroscopy. Furthermore, the properties of **2** can be tuned by protonation, alkylation, oxidation and coordination to metal centers.



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Photochromic Triads for All-Optical Logic Gates

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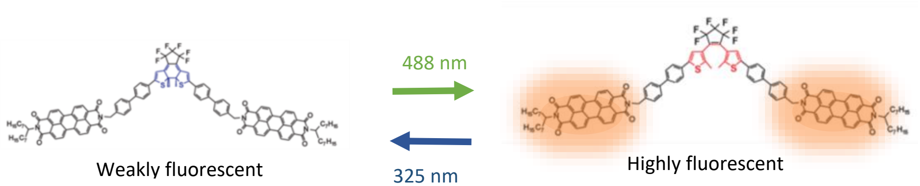
The ongoing challenge to miniaturize electronic devices pushes common lithography techniques to their limits. For the alternative development of optoelectronic components, photochromic molecules are promising candidates, especially for optical data processing. [1] Photochromic molecules can be converted between two bistable forms by light, which is accompanied by a change of their optical and electronic properties. The state of the photochromic unit can then be monitored by the emission of two covalently linked chromophores. For applications in optoelectronic devices however, such photochromic molecules need to have a high photostability, a high fatigue resistance as well as a promt response to the incident light. To gain insights into these requirements, a thorough analysis of the switching behavior of photochromic molecules is necessary. Therefore, we study the fluorescence modulation, that results from switching the photochromic molecule between its two states. While earlier work demonstrated the transistor function of photoswitches on an optical level [2], we are aiming to realize an all-optical logic gate with photochromic molecules.



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Polymer Composite Films for Thermoelectric Application

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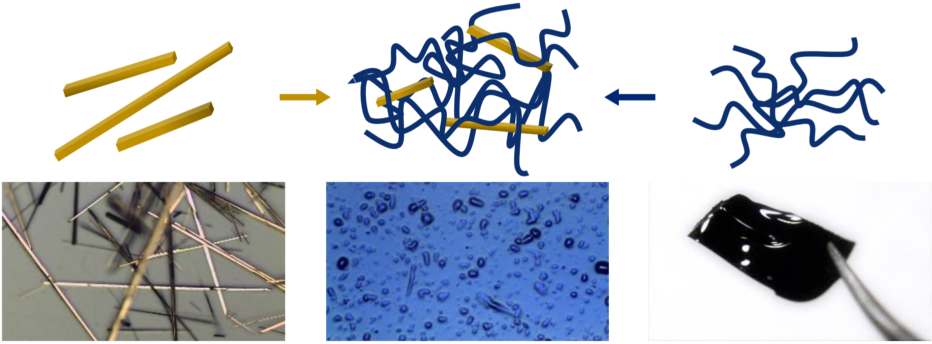
Because of their great potential in power generation from waste heat, thermoelectric materials have become of great interest in energy research. In recent years the focus has largely shifted from inorganic semiconductrors to organic materials as a low-cost, sustainable alternative.
A measure for the efficiency of converting waste heat into electrical power is the thermoelectric figure of merit $zT = \sigma S^2 T/\kappa$. To get sufficiently high zT values for application, the electrical conductivity σ of the film needs to be maximized, while minimizing its thermal conductivity κ. Low-dimensional organic metals are characterized by a metallic conductivity behavior over a wide temperature range [1], therefore exhibiting superior charge carrier transport. Polymers on the other hand lack high electrical conductivty as a result of their inherent disorder but show sufficiently low thermal conductivty and are easily solution processed at large scales. Here both material approaches are combined by preparing composite films of the well studied polymer PEDOT:PSS blended with crystallites of the low-dimensional molecular metal TTT_2I_3.
First results on the thermoelectric properties of these polymer-molecule composites will be presented and evaluated with respect to their application potential in thin film based thermoelectric generators.



TTT_2I_3

composite film

PEDOT:PSS

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Optoelectronic Properties of $Cs_2AgBiBr_6$ Thin Films: The Influence of the Precursor Stoichiometry

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$Cs_2AgBiBr_6$ is a promising candidate in the search for lead-free alternatives for perovskites to be applied in solar cells. However, thin film solar cells comprising this material have not been able to exceed 2.5 % power-conversion efficiency so far, which can be related to factors such as inefficient exciton formation, the large and indirect bandgap and a high trap density.[1][2][3][4]

In order to address these issues, we investigate the influence of the precursor stoichiometry on the optoelectronic properties of this material in thin films. We show that by working with an excess of AgBr combined with a deficiency of $BiBr_3$, the films show a significant increase in preferred orientation while remaining almost phase pure.

Moreover, steady state photoluminescence measurements show higher emission intensity, time-resolved photoluminescence measurements show an extended charge carrier lifetime, while time-resolved microwave conductivity (TRMC) measurements reveal an increase in the charge carrier mobility. These effects altogether lead to an increase in the power-conversion efficienciy (PCE) of the resulting solar cells, associated with higher values for V_{OC}, *FF* and J_{SC}.

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New generation 2D-Hybrid perovskites incorporating organic semiconductor layers

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In the field of photovoltaics, hybrid metal halide perovskites have demonstrated strong potential as they surpassed power conversion efficiencies (PCEs) of 22% within a few years of research [1]. Tremendous progess regarding PCE and stability has been made by changing the material composition from the initial methylammonium lead triiodide perovskites ($CH_3NH_3PbI_3$ = MAPI) to mixed cation and mixed halide systems such as $FA_{1-x}MA_xPb(I_{1-y}Br_y)_3$, where FA stands for formamidinium ion [2,3]. Nevertheless, there are some fundamental issues such as thermal and photostability which need to be studied in detail. Especially, the influence of internal interfaces on photophysics, charge generation, charge separation as well as the dimensionality (2D vs. 3D) still need to be understood and correlated with the underlying preparation method. Lower dimensional perovskites, such as the Ruddlesden-Popper phase, are obtained by introducing alkylammonium cations, such as butylammonium (BA) or phenetylammonium (PEA), which are not able to occupy the interstitial position (similar to MA), which is limited to 2.6 Å for 3D perovskites [4]. Even though layered perovskites exhibit excellent environmental stability, the overall photovoltaic performance can often be poor due to the preferential parallel orientation of the semiconductor layer and the insulating nature of the longer alkylammonium cations, which result in an inherent anisotropy of charge transport [5]. Here we highlight the potential of incorporating tailored, optoelectronically active ammonium cations from the family of diketopyrrolopyrroles, rendered with appropriate energy levels that match those of the inorganic layers, instead of using photo-inactive ammonium ligands.

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Electrochemical and photochemical CO_2 reduction catalyzed by metal porphyrins

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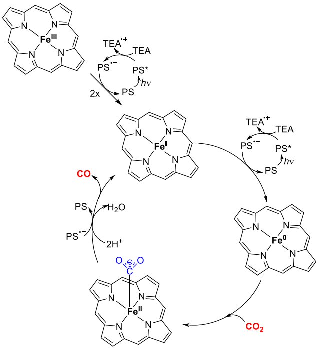
Carbon dioxide is of great industrial interest due to its applicability as renewable C1 feedstock for various chemicals as well as energy storage. Fixation of carbon dioxide could solve problems regarding global warming, increasing energy demand and depletion of fossil fuels. Since CO_2 reduction is an energy demanding process, efficient and selective catalysts have to be investigated. Herein we report both the electrochemical and the photochemical carbon dioxide reduction catalyzed by metal porphyrins. Furthermore, we studied the influence of different metal centres, effect of positively charged moieties and solvents on the catalytic activity. For photochemical reduction we also investigated the impact of different photosensitizers on the reaction.



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Copper Complexes of Bis(pyrazol-1-yl)acetic Acids

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Copper-dioxygen reactions have aroused more and more attention in recent years due to their remarkable reaction properties observed in nature.[1] Thus, we previously reported on a dinuclear cupric complex $[Cu^{II}_2(bd\textit{t}bpza)_2(NO_3)_2]$ bearing the κ^4-*N,N,O,O-* coordinating bis(3,5-di-*tert*-butylpyrazol-1-yl)acetato ligand (bd*t*bpza).[2,3]

To further investigate structural and functional models of dinuclear type 3 copper enzymes, we synthesized the heteroleptic cuprous compounds [Cu(Hbd*t*bpza)Cl] (**1**) as well as [Cu(Hbdppza)Cl] (**2**), bearing the more sterically demanding *N*,*N*,*O*-heteroscorpionate ligands in a κ^2-*N,N* coordination mode. X-ray structure determination of **2** revealed a trigonal planar coordination geometry of the copper center. Exposure of the cuprous complexes to air led to the activation of dioxygen. Hereby, **1** was converted to the cupric $[Cu^{II}_2(Obd\textit{t}bpza)_2]$ complex by an intramolecular C-H activation, resulting in a self-hydroxylation on the *tert*-butyl moiety. Complex **2**, however, was oxidized to result in the homoleptic bisligand complex $[Cu^{II}(bdppza)_2]$, with the release of H_2O_2 as a byproduct. In order to obtain more insight into the mechanisms of oxygen activation, DFT-calculations of the presumable dinuclear Cu^{II}-μ-η^2:η^2-peroxido- and Cu^{III}-bis-μ-oxido-intermediates have been performed.

Additionally, we present promising preliminary results regarding the electrocatalytical hydrogen evolution reaction (HER) by the homoleptic cupric complexes $[Cu(bd\textit{t}bpza)_2]$, $[Cu(bdmpza)_2]$ and $[Cu(bpza)_2]$.

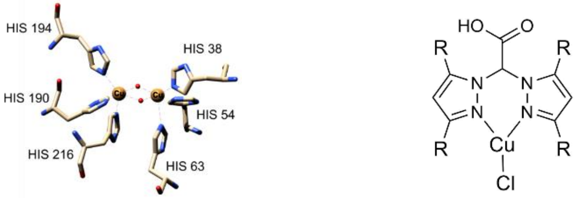

Figure 1: Left: Tyrosinase as an example of a dinuclear type 3 copper enzyme (PDB 3AWV). Right: Cuprous complexes bearing bis(3,5-disubstituted pyrazol-1-yl)acetic acids (with R = ^{t}Bu (**1**), Ph (**2**)).

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Photocatalytic Properties of Self-Organized Organic-Inorganic Hybrid Nanostructures

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Organic and inorganic materials combined in one hybrid architecture cover a large set of promising application fields reaching from solar cells to photocatalysts. For assembling the two material classes, either covalent bonds or supramolecular interactions can be exploited. The latter case mainly avoids synthetic effort making these structures facile and cost-efficient in their fabrication. Nanoscaled cadmium sulfide capped with poly(acrylic acid) (PAA) offers the opportunity of further systematic modification via electrostatic self-assembly: Combination with the tetravalent 5,10,15,20-tetrakis(4-trimethylammonio-phenyl) porphyrin (H_2TAPP) and its zinc metalated derivative (ZnTAPP) forms aggregates with high potential in photocatalysis and as pigments in quantum dot sensitized solar cells. The photocatalytic properties of the system have been demonstrated based on the model reaction, where the metal center and the polymer chain length played a key role.

To circumvent photobleaching an assembly of two inorganic nanoparticles provides a significantly higher stability. The functional groups of the polymers can serve as anchor groups for semiconducting nanoparticles, which can be synthesized in the same reaction flask, as the previous reaction does not form side products. This hierarchical built-up catalyst can pave the way to novel catalyst systems based on supramolecular interactions.

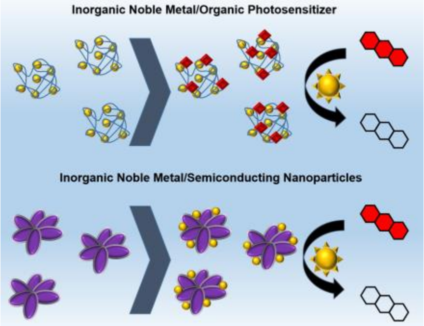

Figure 1. Two hierarchically built hybrid nanoparticle systems based on supramolecular interactions for solar energy conversion.

Germanium-based nanostructure synthesis guided by amphiphilic diblock copolymer templating

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Latest research in the field of hybrid photovoltaics focuses on the benefits of inorganic and organic materials. Flexibility, low cost and large-scale production are the most valuable properties of organic components whereas the inorganic components add chemical and physical stability. So far thin films based on titanium dioxide are well investigated, whereas less is known about germanium-based compounds.[1] In this work, we analyze thin films with optical, electrical and morphological measurement techniques to understand and control the corresponding properties. An amphiphilic diblock copolymer templating with polystyrene-b-polyethylene oxide (PS-b-PEO) and a metal-semiconductor precursor are used to prepare thin films via sol-gel synthesis. The copolymer templating results in nanoporous foam-like germanium-based thin films. In the present study, different molar concentrations of germanium-based compounds are prepared and analyzed. The focus is to find the best compound ratio and set new benchmarks for hybrid photovoltaic applications.

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Energy Release of Metastable Quadricyclane Mediated by Photoexcitation of Rylene Dyes

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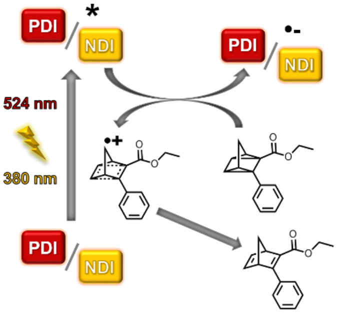
Due to its high energy storage density and the elimination of disadvantages like unsuitable absorption properties and low quantum yields by the modification of the carbon scaffold, norbornadiene-quadricyclane photoswitches are unarguably the most promising candidates of all molecular solar thermal (MOST) storage systems.[1] The high kinetic stability of quadricyclane, which is caused by an activation barrier of 140 kJ/mol for the cycloreversion to norbornadiene, is on the one hand causing a long half-life time of the storing fluid but also hampers an simple energy release.[2] To deliberately induce this process oxidative catalysis was found to be highly promising. Several pathways have been reported to create the structurally labile QC cation radical which undergoes irreversible isomerization to NBD, including the irradiation of n-type semiconductors like CdS and TiO_2 in the presence of quadricyclane.[3] In our research we investigated the use of a variety of irradiated rylene dyes, namely NDIs and PDIs, to trigger the rearrangement of QC derivatives to their corresponding NBD isomers. Furthermore new NBD-NDI hybrids were synthesized by linking both building blocks covalently in various fashions. This new class of molecules was investigated in regards of their optical properties and their behavior during photoexcitation.



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Tailoring Electronic Order in Supramolecular Architectures to Control Exciton Transport Characteristics

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Self-assembly of molecular building blocks into supramolecular aggregates provides an attractive route to design well-defined architectures with novel functionalities. For instance, we have recently shown that single supramolecular nanofibers based on a carbonyl-bridged triarylamine core feature unprecedented exciton transport characteristics over distances of more than 4 µm at ambient conditions.[1]

Here, we demonstrate that the self-assembly of a carbonyl-bridged triarylamine derivative in two different solvents results in supramoelcular architectures with different morphological and optical features. Morphological studies show that in these solvents either single supramolecular nanofibers or supramolecular nanofiber bundles are formed. Optical studies reveal that in both solvents H-aggregates (in with individual monomers are aligned cofacially) are present, yet, with distinctly different optical signatures. Notably, for single supramolecular nanofibers, an almost completely suppressed 0-0-transition at room temperature was found, indicating high electronic order and strong electronic coupling, which paves the way towards perfect H-aggregates. For nanofiber bundles, in contrast, this electronic order is less pronounced.

We directly visualize micrometer long exciton transport by combining photoluminescence microscopy with detection-beam scanning and time-correlated single-photon counting. By increasing the electronic order via the supramolecular architecture we enhance the exciton diffusivities by up to one order of magnitude.

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In situ printing of active layers of PBDB-T-SF:IT-4F for application in high-efficiency organic solar cells

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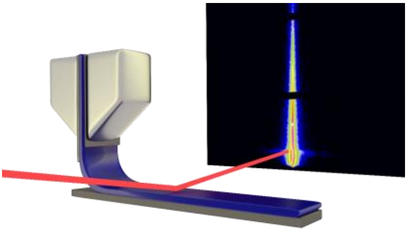
Organic solar cells are a promising alternative to conventional silicon organic solar cells due their high mechanical flexibility, semi-transparency and leight weight which allows new applications of photovoltaics e.g. in buildings, art and clothes. High-efficiency materials have been developed successfully, such as for example PBDB-T-SF: IT-4F, which can achieve a power conversion efficiency of about 13 %. However, towards commmerialization, the main challenge of up up-scaling needs to be overcome. Printing of active layers with a slot-die coater is a promising technique to enable large production of organic solar cells. However, this process of thin film deposition needs to be understood and optimized as the morphology of the active layer has a high impact on the solar cells performance. Therefore, the process of slot-die coating and drying of active layers based on PBDBT-SF:IT-4F were studied in situ with optical microscopy, UV/Vis spectroscopy and grazing incidence small angle X-ray scattering (GISAXS) to get insights into the morphology formation.



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Developing descriptors for the prediction of adsorption energies on metal oxides

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On transition metals, first-principles based reductionist microkinetic models are successfully employed to computationally screen for promising new transition metal (TM) and TM alloy catalysts. Next to the general Sabatier principle, these models primarily root on an exploitation of Brønsted-Evans-Polanyi (BEP) relations [1] and linear scaling relations [2]. The prior relate activation barriers to (computationally more accessible) thermochemical adsorption energies. The latter relate adsorption energies of classes of reaction intermediates, ultimately reducing the required first-principles input to the microkinetic model to a small number of key adsorption energies.

Fundamentally, linear scaling relations arise at TM catalysts as a consequence of the *d*-band dominated electronic structure. Already, this linearity is only approximate, with outlier adsorption energies easily deviating from the trend by up to 1 eV. At other materials classes, deviations can be even more significant, calling for improved approaches that yield reliable adsorption energies at still comparably low computational cost (i.e. demanding an equal or lower amount of computationally intensive first-principles calculations). To this end, we have recently demonstrated the usefulness of a compressed sensing approach for TM and TM alloy catalysts. The corresponding SISSO (sure independence screening and sparsifying operator) approach allows to predict the adsorption energies from descriptors that are expressed as nonlinear functions of intrinsic properties of the clean catalyst surface (so-called primary features), e.g. coordination numbers, d-band moments, and density of states at the Fermi level. Here, we extend this approach to TM oxide catalysts and oxygen evolution catalysis. Next to establishing a systematic first-principles database for the SISSO training, a key aspect of our work is to identify primary features for this class of materials.

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Influence of Morphology on the Density of Charge-Transfer States in Organic Donor/Acceptor Blends

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Organic small molecule solar cells are used as a test bed to investigate the influence of film morphology on the density of charge-transfer (CT) states. CT states are considered as precursors for charge generation and their energy (E_{CT}) as the upper limit for the open-circuit voltage (V_{OC}) in organic donor/acceptor solar cells. In this study the influence of morphology for two perylene donors (crystalline DIP versus amorphous DBP) with almost identical ionization energy is investigated. As acceptor material the fullerene C_{60} is used.

By combining device measurements with optical and low-energy ultraviolet photoelectron spectroscopy, a comprehensive picture is obtained that describes how morphology and the connected density of states (DOS) affect device performance and the spectroscopic signature of CT states. Especially for the crystalline donor material DIP strong exponential tail states reaching far into the gap are observed, which can be related to the presence of grain boundaries. A voltage dependent filling of these states is identified as the origin of a blue shift of electroluminescence (EL) spectra with increasing applied voltage.

Different approaches [1-3] are compared to study the influence of static and dynamic disorder in the description of CT emission and absorption spectra of organic solar cells. Despite the fact that both donors yield almost identical E_{CT} (and, thus, the same V_{OC}) the Stokes shift between EL and EQE spectra and, concomitantly, the width of the CT DOS varies by more than a factor of 2. We discuss this observation in terms of the donor-acceptor reorganization energy (λ) as well as an additional contribution of static disorder (σ). Remarkably, the more crystalline donor DIP shows a signifant contribution of the latter, while for the amorphous DBP this additional term is not required. This highlights the importance of film morphology in organic solar cells.

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Suppression of Hysteresis in Perovskite Solar Cells by Reducing Ionic Migration

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Despite the rapid development of perovskites solar cells (PSCs), it is still urgent to address problems such as hysteresis and photo/electrical field induced degradation, to further improve efficiency and reliable of PSCs. It is known that the ionic migration is critical for these detrimental behaviors, yet, direct in-situ studies are still lacking to elucidate the kinetics of the ionic migration. We study the ion migration behavior in $CH_3NH_3PbI_{3-x}Cl_x$ films by employing photoluminescence imaging microscopy to in-situ investigate both its spatial and time-dependent changes.[1] We fabricate PSCs incorporating phenyl-C61-butyric acid methyl ester (PCBM) and PCBM-polymer to investigate the influence of diffusion of PCBM and a potential interdiffusion into the perovskite film on the hysteretic behavior. We observe the migration of iodine/vacancies under an external electrical field in three systems: (1) single perovskite layer (2) perovskite/PCBM bilayer with PBCM molecules viable to diffuse (3) perovskite/PCBM-polymer bilayer, where the fullerene molecules are attached to a polymer backbone impeding diffusion. The results from step-wise temperature dependent chronoamperometric measurements demonstrate the reduction of migration and increase of activation energy when involved with PCBM molecules. Using X-ray photoelectron spectroscopy, we observe that PCBM molecules may diffuse into a perovskite film and passivate iodine related defects in the material, not only at the interface. This passivation significantly reduces the ionic migration, leading to the reduction of modulation of built-in field and interfacial barriers in devices. Our study furthermore corroborates that the suppression of iodide ion movement is key to improve the performance and stability of PSCs.

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