

e-conversion

Conference Venice 2019

September 9-13, 2019



In cooperation with Venice International University (VIU)

Welcome

General Information

Welcoming Message

We are happy to welcome you to the first international **e**-conversion conference to be held at Venice International University (VIU), San Servolo, Italy from September 9 – 13, 2019.

e-conversion is a new Cluster of Excellence funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy. The cluster unites more than 40 Principal Investigators and their research groups from the Technische Universität München (TUM) and the Ludwig-Maximilians-Universität München (LMU), as well as from Max Planck Institutes in Stuttgart and Mülheim an der Ruhr. Together, the researchers investigate the fundamental processes involved in the conversion of renewable energies.

Whether it is photovoltaics, photocatalysis, or batteries, the interfaces between different materials always play a key role. The physical processes at interfaces can result in unwanted energy losses, resistances, overpotentials or degradation - but are simultaneously the key to performance. Hence, the design of the interfaces and a thorough understanding of these elementary processes is crucial for the efficiency and durability of energy conversion technologies. **e**-conversion therefore merges the powerful concepts of nanoscience and mechanistic energy research to create well-defined and tunable reference systems, and to es-

tablish fundamental understanding through their comprehensive (operando) characterization.

With this grand kickoff conference, we wish to foster scientific exchange between the members of the cluster and renowned scientists from around the globe. The talks shall also give the graduate students of **e**-conversion an overview of current research topics on fundamental research concerning energy conversion processes. In addition to the talks, the students will present more than 50 posters at two poster sessions.

We trust that the enchanting atmosphere of the beautiful island of San Servolo in the Venetian Lagoon will stimulate many discussions between speakers and participants. A majority of the 40 PIs involved within **e**-conversion will be present at the conference, ensuring a broad and stimulating audience.

We wish you all an inspiring and fruitful meeting.

Thomas Bein, Jonathan Finley, Ulrich Heiz, Katharina Krischer, Dario Leister, Bettina Lotsch, Karsten Reuter, Thomas Weitz
(Executive Board of **e**-conversion)

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Contact

Venue

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Venice International University

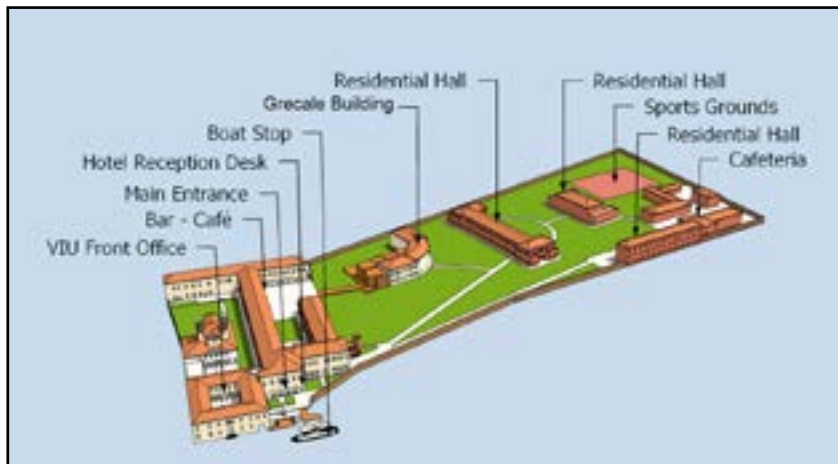
- Conference Venues -

Monday - Wednesday and Friday

Talks	Aula Magna
Coffee breaks	Lobby
Welcome reception	Lobby
Poster session I	Lobby

Only on Thursday

Talks	Auditorium
Poster session II	Grecale Building
Coffee breaks	Grecale Building
Conference dinner	Grecale Building



Timetable Vaporetto (Water Bus) Line No. 20

LINEA 20

S.ZACCARIA - S.SERVOLO - S.LAZZARO - LIDO CASINÒ and back

	08:05			08:35			09:05			13:30			14:15		
LIDO Casinò	06:55	07:20	07:45	08:15	08:45	-	09:15	09:45	10:30	11:10	11:50	12:30	13:10	-	13:55
S.MARCO-S.ZACCARIA "B"	07:05	07:30	07:55	-	08:25	-	08:55	-	09:25	09:55	10:40	11:20	12:00	12:40	13:20
S.SERVOLO	-	07:35	08:00	08:10	08:30	08:40	09:00	09:10	09:30	-	10:45	-	12:05	-	13:25
S.LAZZARO	-	07:40	-	08:15	-	08:45	-	09:15	09:35	-	10:50	-	12:10	-	13:40
S.SERVOLO	07:15	07:50	-	08:25	-	08:55	-	09:25	09:45	10:05	11:00	11:30	12:20	12:50	-
S.MARCO-S.ZACCARIA "B"	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
LIDO Casinò	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

	17:30			18:15			19:00			(A)	(A)	(A)	(A)	(A)
LIDO Casinò	14:40	15:15	15:45	16:10	16:35	17:10	-	17:55	-	18:40	-	19:40	20:30	21:30
S.MARCO-S.ZACCARIA "B"	14:50	15:25	15:55	16:20	16:45	17:20	-	18:05	-	18:50	-	19:50	20:40	21:40
S.SERVOLO	14:55	15:30	-	-	16:50	17:25	17:35	18:10	18:20	18:55	19:05	-	-	-
S.LAZZARO	15:00	15:35	-	-	16:55	-	17:40	-	18:25	-	19:10	-	-	-
S.SERVOLO	15:10	15:45	16:05	16:30	17:05	-	17:50	-	18:35	-	19:20	20:00	20:50	21:50
S.MARCO-S.ZACCARIA "B"	-	-	-	-	-	-	-	-	-	-	-	-	-	-
LIDO Casinò	-	-	-	-	-	-	-	-	-	-	-	-	-	-

(A) = Stop at S.LAZZARO on request

EMERGENCY CALLS

Ambulance: 118

Fire Department: 115

Police: 112 / 113

Mobile phone of the e-conversion team

(Silke Mayerl-Kink, Dr. Peter Sonntag, Dr. Birgit Ziller)

+49 152 01 53 51 20

DISCLAIMER

The organizers do not hold any liabilities on damages, losses, health issues, etc.. All participants are advised to take care about their travel and health insurances related to this conference.



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Mon, 9:45 a.m.

COMPOSITION AND INTERFACE ENGINEERING OF PEROVSKITE SOLAR CELLS

Anders Hagfeldt

Laboratory of Photomolecular Science, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 22 % with a mixed composition of iodide/bromide and organic and inorganic cations. Recently, we have managed to find efficient compositions avoiding bromide and methyl-ammonium. With the use of SnO_2 compact underlayers as electron acceptor contacts we have constructed

planar perovskite solar cells with a hysteresis free efficiency above 20 %. Through the compositional engineering larger perovskite grains grown in a monolithic manner are observed and reproducibility and device stability are improved. With regards to lifetime testing, we have shown a promising stability at 85 °C for 500 h under full solar illumination and maximum power

point tracking (95 % of the initial performance was retained). Recently, we have also commented on the standardization of PSC aging tests.

Mon, 10:30 a.m.

SEMICONDUCTOR NANOWIRES FOR THERMOELECTRIC ENERGY CONVERSION

Gregor Koblmüller

Walter Schottky Institute and Physics Department, Technical University of Munich, Germany

Thermoelectric energy conversion (TEC), which relies on the conversion of temperature gradients into electricity or vice versa, has attracted a lot of attention for applications in waste heat recovery for power generation and in solid-state refrigeration. The prime challenge is to improve the conversion efficiency by adapting suitable materials with large thermoelectric power factor ($S^2\sigma$) and low thermal conductivity (κ). Semiconductor nanowires (NWs) are such promising materials, since they can decouple the undesired interdependencies between thermoelectric parameters commonly seen in bulk mate-

rial. As 1D-like carrier channels, NWs can further exploit quantum-confinement enhanced electronic density of states (DOS) along with significant phonon boundary scattering necessary for improved TEC performance.

Here, we present our recent progress in the exploration of high carrier-mobility III-V based NWs for TEC. We first illustrate the influences in carrier mobility and density of high-mobility InAs NWs by doping and crystal phase engineering [1], and show how these affect the corresponding thermo-power [2]. We further explore

sophisticated core-shell NW systems with strongly 1D-confined carrier channels. In particular, modulation-doped GaAs-AlGaAs core-shell NWs in field-effect transistor test structures [3] are demonstrated to exhibit 1D-subband transport with discrete step-wise conductance [4], which leads to strong quantum oscillations in thermopower [5]. The core-shell structures further yield strong reductions in thermal conductivity that are about one order of magnitude lower than state-of-the-art GaAs NWs [5].

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Mon, 11:30 a.m.

IONIC AND ELECTRONIC CHARGE CARRIERS IN SOLIDS: IMPLICATIONS FOR ENERGY CONVERSION AND STORAGE

Joachim Maier

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Solid State Ionics provides the basis for a deeper understanding of electrochemical energy storage and applications such as batteries and fuel cells [1]. This is due to the fundamental role of ionic and electronic point defects as relevant charge carriers and reactive centers. It is shown how and by which adjusting screws their contributions can be tuned. Of special relevance is the situation at interfaces (“nano-ionics”). Here redistribution phenomena occur that are paramount for the

understanding of transport, transfer and storage.

The significance of these considerations exceeds the realm of electrochemical applications [2,3]. Their relevance for fields such as heterogeneous catalysis, solid state reactions, semi- and superconductor science has been explored in recent works. As an example of current interest, “photo-perovskites” are addressed [4].

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Mon, 12:15 p.m.

USING COMPUTATION TO GUIDE ENERGY MATERIALS DISCOVERY

Ram Seshadri

Materials Department, University of California Santa Barbara, CA 93106

Materials play a critical role in advancing clean-energy technologies, but oftentimes, finding the best materials for a task can require extensive experimentation. With improvements in the reliability and speed of computational methods, it is increasingly of interest to screen materials computationally, before they are tested. Two classes of materials applications will

be described where computation plays a great role in the search for higher-performing materials. The first is in the area of magnetocalorics, which are materials that display great promise for refrigeration and waste-heat recovery. The second is the area of photovoltaic materials that directly convert sunlight into electricity.

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Mon, 2:30 p.m.

UNDERSTANDING DEFECT PHYSICS TO STABILIZE METAL-HALIDE PEROVSKITE SEMICONDUCTORS FOR OPTOELECTRONIC APPLICATIONS

Annamaria Petrozza

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Semiconducting metal-halide perovskites present various types of chemical interactions which give them a characteristic fluctuating structure sensitive to the operating conditions of the device, to which they adjust. This makes the control of structure-properties relationship, especially at interfaces where the device realizes its function, the crucial step in order to control devices operation. In particular, given their simple processability at relatively low temperature, one can expect an intrinsic level of structural/chemical disorder of the semiconductor which results in the formation of defects.

Here, first I will summarize our understanding of the nature of defects and their photo-chemistry, which leverages on the

cooperative action of density functional theory investigations and accurate experimental design. Then, I will show the correlation between the nature of defects and the observed semiconductor instabilities. Instabilities are manifested as light-induced ion migration and segregation, eventually leading to material degradation under prolonged exposure to light.

Understanding, controlling and eventually blocking such material instabilities are fundamental steps towards large scale exploitation of perovskite in optoelectronic devices. By combining photoluminescence measurements under controlled conditions with ab initio simulations we identify photo-instabilities related to competing light-induced formation and annihilation of trap states, disclosing their characteristic length and time scales and the factors responsible for both processes. We show that short range/short time defect annihilation can prevail over defect formation, happening on longer scales, when effectively blocking undercoordinated surface sites, which act as a defect reservoir. Finally, based on such knowledge, I will discuss different synthetic and passivation strategies which are able to stabilize the perovskite layer towards such photo-induced instabilities, leading to improved optoelectronic material quality and enhanced photo-stability in a working solar cell.

Mon, 3:15 p.m.

UNDERSTANDING AND ENHANCING ION TRANSPORT IN SOLIDS AND AT INTERFACES FOR ALL-SOLID-STATE LITHIUM AND SODIUM ENERGY STORAGE

Linda F. Nazar, L. Zhou, K. Kaup, Z. Zhang, K.-H. Park

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Single-ion conducting solid electrolytes are gaining tremendous attention as essential materials for solid-state energy storage. While the ability to utilize such “fast-ion conductors” relies on formation of efficient nanocomposites for the electrode, the discovery and design of new and advanced materials in this class hinges on understanding their intrinsic nature. Comprehensive knowledge of the factors that dictate facile ion transport still remains elusive, as does mastering the interface of the solid electrolyte with the electrode materials.

This presentation will examine the challenges, and ways to address these factors with new Li-ion and Na-ion conductors in

the crystalline and glassy alkali thiophosphate families, while also shedding light on new design concepts for ion transport and electrolyte-electrode interfaces. The talk will cover an overview of the challenges and recent findings in our laboratory. Significant increases in the conductivity of several materials will be presented that have been attained by both tuning composition, and developing scalable routes to create materials that exhibit the necessary fast ion conductivity together with good chemical stability.

An understanding of superionic conductivity in these alkali thiophosphates has been achieved using a combination of structural elucidation, the maximum entropy method

(MEM), solid state NMR studies, and ab initio molecular dynamics simulations. We correlate structure with ionic conductivity to understand how cation disorder and a frustrated energy landscape affects the conductivity and activation energy.

Mon, 4:30 p.m.

HOW DOES MOLECULAR STRUCTURE INFLUENCE CHARGE MOBILITY? MINING A DATABASE OF ORGANIC SEMICONDUCTORS

Harald Oberhofer

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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 wide-scale adoption are their low intrinsic charge carrier mobilities.

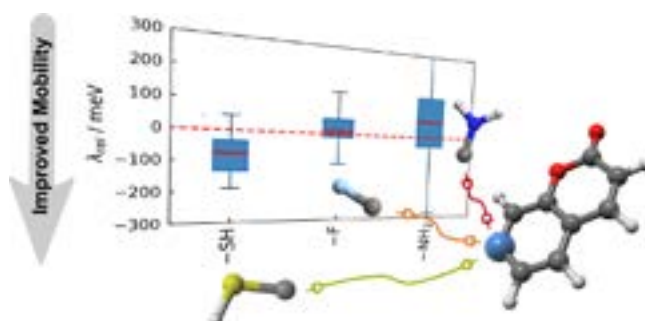
Improving these is usually attempted by structural tuning of a promising compound family, thereby relying on intuition, experience, or simply trial and error. While sometimes quite successful, such incremental changes only lead to a local exploration of the potentially vast chemical space of possible 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.

We carry out such an analysis of the charge carrier mobilities of > 64,000 or-

ganic crystals initially extracted from the Cambridge Structural Database (CSD) and screened for charge transport properties using first-principle derived descriptors. Thereby, our screening already recovers many known and well performing materials, at the same time showing a large number of heretofore-unknown promising candidates, not yet considered for organic electronics applications.

Furthermore, we evaluate the contributions of molecular scaffolds and side groups to the charge transport descriptors of each crystal contained in our database, to reveal statistically reliable, general design criteria. 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.

Thus, the network analysis can point towards promising yet so-far overlooked theoretical and experimental design routes for organic electronics materials.

Tue, 9:35 a.m.

UNDERSTANDING AND INFLUENCING STRUCTURAL EVOLUTION IN MORPHOLOGICALLY COMPLEX SEMICONDUCTORS FOR PHOTOVOLTAIC APPLICATIONS

N. C. Davy, M. Sezen-Edmonds, X. M. Zhao and Yueh-Lin Loo

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I will highlight two examples in which understanding the molecular interactions has allowed us to impart exquisite structural control to semiconductor thin films, leading to improved opto-electronic properties.

(a) Contorted chromophores lead to see-through solar cells with scalable power production:

Crystallinity has long thought to be critical for long-range charge transport. But polycrystalline thin films often exhibit defects, such as grain boundaries, that can trap charge. Contrary to convention, we have employed conformationally contorted organic chromophores that deposit as amor-

phous thin films as active layers in organic solar cells. Because these amorphous films are pinhole-free, we demonstrate power production that scales linearly with active-layer footprint. These wide band-gap chromophores absorb ultra-violet light exclusively, resulting in see-through solar cells with high optical transparency [1].

(b) Vertically orienting layered perovskites to enhance performance and stability of hybrid photovoltaics:

While 2D hybrid organic-inorganic perovskites are more resilient against humidity and oxygen, these materials have thus far resulted in solar cells that consistently underperform compared to their

3D counterparts. Vertically orienting the alternating organic and inorganic layers in 2D perovskites active layers can reduce charge transport resistance and improve solar-cell performance. Here, I will describe a simple and robust post-deposition processing procedure to induce large-scale reorientation of grains in polycrystalline 2D perovskite thin films. This procedure is generalizable across a broad class of 2D perovskites with different chemistries, structure (i.e., Dion-Jacobson versus Ruddleson-Popper), and composition, resulting in solar cells with higher efficiencies and substantially improved stability [2].

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Tue, 10:20 a.m.

NANOZYMES: NANOPARTICLES THAT MIMIC ENZYME ARCHITECTURE FOR THE OXYGEN REDUCTION REACTION AND THE CARBON DIOXIDE REDUCTION REACTION

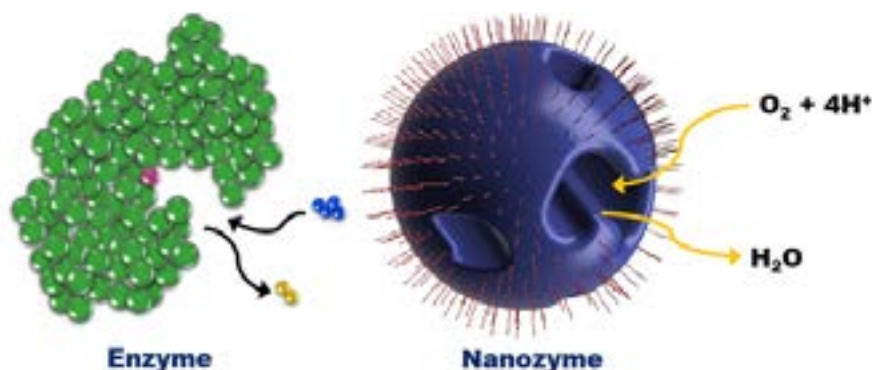
T. M. Benedetti¹, P. Wilde², P. O'Mara¹, J. Wordsworth¹, C. Andronesco², S. Cheong¹, R. D. Tilley¹, W. Schuhmann², J. Justin Gooding¹

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Nanoparticle electrocatalysts and enzymes present common features such as their size and the reactions they catalyze. One main difference between them is that while the active sites of nanoparticles are in direct contact with the electrolyte, enzymes have their catalytic sites spatially separated from the solution environment, providing high reaction kinetics and selectivity.

It is expected that such an approach applied to nanoparticles design can influence both the electronic properties of the catalytic site [1] and the transport of reactants and products [2,3] with benefits to the electrocatalytic performance. Thus, in this work the enzyme architecture is used as inspiration to make nanozymes [4]: nanoparticles containing isolated channels and with the outside surface electrochemically passivated to enable the electrochemical reaction to happen exclusively inside those channels. With that, it was able to study the effect of



having an electrocatalytic reaction happening in a different solution environment of the bulk electrolyte, like in an enzyme. Among the different possibilities, PtNi nanoparticles for the oxygen reduction reaction (ORR) was chosen as a concept model for this study.

The nanozymes presented improved ORR activity with respect to both spherical nanoparticles and mesoporous nanoparticles that have interconnected pores instead of isolated channels. A dependence

of the channels size was also observed: nanozymes with smaller channels are more active than the nanozymes with larger channels at lower overpotentials. With increasing overpotential, the nanozymes with larger channels become more active than the ones with smaller channels. These results shine light into the origins of the improved ORR activity inside those confined environments.

Subsequently we show how nanozymes can be developed for performing cascade reactions using the carbon dioxide reduction reaction as the model reaction where nanoparticles with a silver core and a copper shell are designed.

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Tue, 11:35 a.m.

ELECTROCHEMICAL CONVERSION OF SUSTAINABLE ENERGY

Ib Chorkendorff

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In this presentation, I will give an overview of some of our recent progress in making nanoparticles alloys in relation to electrochemical conversion of sustainable energy [1]. In the first case it will be used to elucidate size dependence and efficiency for catalysts related to the Water splitting i.e. Hydrogen- and in particular Oxygen-evolution reaction (OER) which is the limiting reaction and evaluate the scalability of scarce and expensive elements like the Pt-group metal under acidic conditions [2-4].

We shall discuss caveats of testing catalysts for water splitting [4] and investigate size dependence and isotope labelled experiments will be presented for NiFe nanoparticles for oxygen evolution under alkaline conditions [5]. Here we shall demonstrate a new principle for dynamic detection of gas evolution [6] allowing for a clear distinction between redox states and actual OER [7]. The same principles will be used to demonstrate investigation of conversion of CO or CO₂ into valuable

fuels and chemical electrocatalysis [8-11]. Finally, shall we also touch upon electrochemical ammonia productions – facts or dreams [12].

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Tue, 12:20 p.m.

THE ELECTRON SPIN AND CHIRAL MOLECULES - TOGETHER THEY MAKE THE DIFFERENCE

Ron Naaman

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Spin based properties, applications, and devices are commonly related to magnetic effects and to magnetic materials. However, we found that chiral organic molecules act as spin filters for photoelectrons transmission, in electron transfer, and in electron transport.

The new effect, termed Chiral Induced Spin Selectivity (CISS) [1,2], was found, among others, in bio-molecules and in bio-systems. It has interesting implica-

tions for the production of new types of spintronics devices [3,4] and on electron transfer in biological systems. Recently we observed that charge polarization in chiral molecules is accompanied by spin polarization. This finding sheds new light on enantio-specific interactions and it allows to construct novel methods for enantio-separation [5]. It also opens new ways in interface-spintronics, when chiral molecules are adsorbed on semiconductor surfaces [6].

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Tue, 2:15 p.m.

CONNECTIONS BETWEEN STRUCTURAL DYNAMICS AND OPTOELECTRONIC PROPERTIES OF HALIDE PEROVSKITES FROM FIRST-PRINCIPLES CALCULATIONS

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Halide perovskites (HaPs) are highly promising 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, which challenge our basic understanding of coupling between nuclear vibrations and optoelectronic properties in a semiconductor.

In this talk, I will present our recent explorations of the consequences of the unusual structural phenomena in HaPs for their optoelectronic properties. Theoretical calculations based on density functional theory, molecular dynamics, and tight-binding modeling will be used to examine the impact of structural dynamics on pertinent device-relevant observables. Consequences of the structural dynamics and anharmonicity in HaPs will be discussed for the charge-carrier mobility, Urbach en-

ergy, and defect energetics. It will be shown 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 for energy conversion.

Wed, 9:35 a.m.

A NANOBIENGINEERING APPROACH TO DEVELOPING LIVING PHOTOVOLTAICS

Ardemis Boghossian

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Despite their inspiration in improving synthetic photovoltaics, photosynthetic systems suffer from stabilities and efficiencies that limit their direct use in photovoltaics. While they benefit from autonomous repair and reproduction, photosynthetic systems contain light-harvesting machinery that is optimized for

evolutionary purposes rather than photocurrent production. Herein we present bioengineered cyanobacteria capable of enhanced photocurrent production. We introduce genetically encoded exoelectronic pathways that serve as electron conduits for interfacing photosynthetic cells with nanomaterial scaffolds. These conduits

further enable researchers to electronically rewire the cell metabolism and reprogram biological cells to perform as artificial electronic devices. The ability to improve photovoltaic performance through both nanomaterials engineering and synthetic biology unlocks new possibilities in achieving a viable technology.

Wed, 10:20 a.m.

SN-BASED HYBRID PEROVSKITES: FROM SOLAR CELLS TO HOT ELECTRONS

Maria Antonietta Loi

Photophysics and OptoElectronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG, The Netherlands

Thanks to the intensive research efforts of a large scientific community over the past 10 years, lead-based hybrid perovskite solar cells have reached impressive power conversion efficiency. Against the initial criticism about their instability, also large improvements in the thermal and photo stability of this kind of solar cell were obtained by engineering of their chemical composition, and using robust hole/electron transport layers. Despite these outstanding accomplishments, lead-based compounds are considered not suitable for large-scale production of consumer products.

Among the various alternatives to lead, Sn has been recognized to have a great potential, as the Sn-based hybrid perovskites display excellent optical and electrical properties such as high absorption coefficients, very small exciton binding energies and high charge carrier mobilities. In my talk I will show that Sn-based perovskites display evidences of photoluminescence from hot-carriers with unexpectedly long lifetime [1]. The asymmetry of the PL spectrum at the high-energy edge, is accompanied by the unusually large blue shift of the time-integrated photoluminescence with increasing the excitation power. These

phenomena are associated with slow hot carrier relaxation and state-filling of band edge states.

I will further show all-tin-based hybrid perovskite solar cells with efficiencies of up to 9%. This record result is obtained with the addition of trace amount of 2D tin perovskite, which initiates the homogeneous growth of highly crystalline and oriented FASnI_3 grains at low temperature [2].

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Wed, 11:35 a.m.

DYNAMICS OF CHARGE-CARRIERS AND IONS IN METAL HALIDE PEROVSKITES FOR SOLAR CELLS

Laura M. Herz

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Metal halide perovskites have emerged as attractive materials for solar cells with power-conversion efficiencies rapidly approaching the Shockley-Queisser limit. As trap-mediate charge-recombination becomes less prominent, radiative bimolecular (band-to-band) recombination will dominate, which may be viewed as the inverse of absorption [1].

We show that photon reabsorption inside the hybrid perovskite may effectively reduce charge-carrier losses from thin hy-

brid perovskite films [2,3]. Such photon recycling depends sensitively on film properties and light out-coupling, which may be influenced by device architecture [2]. We show that thin films comprising a quasi-two-dimensional (2D) perovskite region interfaced with a 3D MAPbI₃ perovskite layer allow for highly effective “heterogeneous photon recycling”, because the blue-shifted emission originating from quasi-2D regions overlaps significantly with the absorption spectrum of the 3D perovskite.

This combination fully compensates for the adverse effects of electronic confinement, yielding quasi-2D perovskites with highly efficient charge transporting properties [3]. In addition, we investigate optoelectronic properties of mixed tin-lead iodide and mixed iodide-bromide lead perovskites [4-6]. In the context of silicon-perovskite tandem cells, we discuss the mechanisms underlying detrimental halide segregation in mixed iodide-bromide lead perovskites with desirable electronic band gaps near 1.75 eV [6].

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Wed, 12:20 p.m.

MORPHOLOGY ANALYSIS AND INTERFACE ENGINEERING OF SOLUTION-PROCESSABLE PHOTOVOLTAICS

Tayebeh Ameri

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Organic and Perovskite solar cells are considered as two of the most promising photovoltaic technologies for low cost energy production with the advantages of semi-transparency, flexibility and solution processing. But apart, each still deals with notable challenges to reach their marketing potential and become competitive in their respective field.

The ternary-blend solar cells have been explored in the last decade as a leading strategy in development of organic photovoltaic Technology. Ternary blends with broad spectral absorption have the potential to increase charge generation but feature additional complexity due to unfavorable intermixing and electronic mismatch. Based on a combination of photo physical

analysis, GIWAXS measurements, chemical sensitive imaging methods, and calculation of the intermolecular parameter, here we will discuss how the thermodynamic mixing and energetics of the used components' interfaces are critical design parameters for realizing highly efficient ternary solar cells.

Besides, so far, an enormous progress has been made for perovskite photovoltaics reaching over 23 % power conversion efficiencies. The compositional engineering as well as controlling the crystallization process were key factors in achieving such highly efficient devices. However, fundamental problems, such as the toxicity of hybrid lead halide perovskites, hysteresis and structural instability remain to be

solved for perovskite solar cells. Indeed, the low-temperature solution-processing of perovskite films inevitably causes formation of a certain amount of defects on the surface and at the grain boundaries, which lead to serious trapping, charge accumulation, and recombination problems as well as stability issue. In this work, we will pursue the interface engineering and defects passivation by introducing organic ammonium salts on the perovskite active layer. We will discuss the origin of crystallization changes and performance improvement of treated devices based on the results achieved from optoelectrical and structural investigations.

Thu, 9:35 a.m.

ELECTROCHEMICAL AMMONIA SYNTHESIS

Jens K. Nørskov

Technical University of Denmark

The current industrial ammonia synthesis has a substantial carbon footprint, and an alternative process based on the energy input from sustainable sources, solar or wind would be highly desirable. The

lecture will discuss why alternatives to the Haber-Bosch process are difficult to find and will focus in particular on the possibility of an electrochemical process to reduce dinitrogen.

Thu, 2:15 p.m.

NARROW EMISSION BAND PHOSPHORS FOR APPLICATION IN HIGH-POWER LEDs

Ru-Shi Liu

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Light-emitting diodes (LEDs) are widely used around the world. Scientists are attempting to develop LED devices that do not only have high brightness but also have a high color rendering index (CRI). Phosphor materials play important roles in tuning and optimizing the final luminescent spectrum. Narrow-band emission phosphors must be incorporated into LED chips to achieve high CRI and efficacy. From this perspective, we introduce and discuss key

points in the narrow-band emission spectrum. Three sets of phosphor examples, namely, Eu^{2+} -doped $(\text{Ba}, \text{Sr})\text{Si}_2\text{O}_2\text{N}_2$ [1] and UCr_4C_4 -type [2-10] structures are used to explain these points.

First, we discuss the highly symmetrical local coordination environment of activators, which include cuboid and nine-coordinate structures. Second, we reveal the second shell effect of the substituted

cation channel. Third, we discuss the interaction between the electron from the activator and the vibration from the host lattice (electron-lattice interaction). These model systems help establish and design rules for narrow-band emission phosphors and may guide future studies in discovering potential phosphor candidates for practical applications.

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Thu, 3:00 p.m.

RATIONAL APPROACHES TO ENGINEERING DIRECT ELECTRON TRANSFER IN PHOTOSYSTEM I-BASED BIOPHOTOELECTRODES

Joanna Kargul¹, M. Kiliszek¹, E. Harputlu², M. Szalkowski³, D. Kowalska³, C. G. Unlu⁴, P. Haniewicz¹, M. Abram¹, K. Wiwatowski³, S. Maćkowski³, K. Ocakoglu^{2,5}

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A major bottleneck in the fabrication of efficient biohybrid solar cells and solar-to-fuel devices is the strong charge recombination that is present at the different interfaces forming the complex system. An efficient way to overcome this bottleneck is to add an optimized self-assembled monolayer (SAM) of (bio)organic molecules between the biological photoactive component and the electrode that promotes an efficient direct electron transfer whilst minimising wasteful back reactions.

Another approach is to include plasmonic nanoarchitectures that interact with photoactive components often leading to an improved photocurrent density generated in biophotoelectrodes. Here we show that coupling extremophilic Photosystem I (PSI) reaction centres with

plasmonically active silver island film (SIF) leads to enhancement of both fluorescence intensity as well as photocurrent generation. The nanostructure is assembled by the controlled attachment of PSI to a monolayer graphene deposited on the SIF layer.

The molecular bio-organic interface between PSI and electrode surface is based on: (1) a pyrene-nitrotriacetic acid SAM containing various metallic redox centers, and (2) His-tagged cytochrome c553 monolayer for oriented coupling of the photoactive layer of PSI complexes with the donor side towards the electrode surface. A combination of theoretical calculations, field emission scanning electron microscopy, fluorescence spectroscopy and photoelectrochemical measurements

reveals that the metal center holds the key role for both, the efficient direct electron transfer at the interface and SIF-mediated plasmonic enhancement of fluorescence in the nanostructured PSI layer.

ACKNOWLEDGEMENTS

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Thu, 4:15 p.m.

THE SYNTHESIS OF EXCITONIC GRADE 2D JANUS CRYSTALS

Sefaattin Tongay

Ira A. Fulton Schools of Engineering, Arizona State University, USA

In this talk, I will introduce 2D Janus crystals and discuss one-of-a-kind method for the synthesis of 2D Janus layers discovered by my team at Arizona State University. This new holistic technique enables the synthesis of nearly any 2D Janus

layers at excitonic grade. I will also discuss these synthesis results together with sophisticated scanning transmission electron microscopy (STEM), nano-EELS, and optical spectroscopy techniques.

Thu, 5:00 p.m.

PLASMONIC NANOPARTICLES AS ENERGY CONVERTERS FOR CHEMICAL REACTIONS AND FOR THE LAUNCHING OF ACOUSTIC SURFACE WAVES

Stefan A. Maier

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In addition to the well-established electromagnetic hot spots of plasmonic nanostructures, metal nanoparticles can also act as nanoscale energy transformers from electromagnetic into chemical or acoustic energies. Energetic electron/hole pairs formed via plasmon decay enable control over chemical reactions on the nanoscale, and coherent acoustic vibrations of the nanostructures the controlled launching and detection of acoustic surface waves.

We present our recent efforts to unravel both the energetics and the spatial distribution of hot charge carriers generated in metallic nanostructures via the decay

of localized surface plasmons. Using a combination of bulk electrochemistry and single-particle spectroscopy, we directly determine the energy of hot holes in Au nanocolloids and their energetic contribution to a polymerization reaction at the nanoparticle's surface [1]. Our results demonstrate that the energy contribution of the "hot" holes is maximized upon excitation at the localized plasmon resonance frequency of the particles.

Such plasmon-enhanced chemistry enables further control over nanoscale self-assembly [2] and also a novel super-resolution imaging scheme of optical absorption [3], based on the controlled

cleaving of thiol-bonds via hot electrons excited in top-down fabricated gold nano-antennas. We use this scheme to bridge top-down nanofabrication with bottom-up self-assembly, and further show direct spatial imaging of near-field energy transfer in a Fano cavity.

In addition to hot electron effects, optical excitation of metallic nanoparticles also lead to coherent acoustic vibrations. Using spatially separated source and detector nanoparticles, we demonstrate the launching of acoustic surface waves in the underlying substrate via this scheme [4]. This enables nanoscale interrogation of the properties of surface-acoustic waves.

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Thu, 5:30 p.m.

ADVANCED BATTERIES – ELECTROCHEMISTRY AT INTERFACES AND INTERPHASES

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The electrochemical performance of batteries is determined to a large extent by charge-transfer and charge-transport processes along and across different internal boundaries. Relevant mechanisms range from the deposition of Lithium during charging to aging under high cyclic loading. Mechanistic insights into atomic-scale processes can be obtained by in-operando magnetic resonance – both electron paramagnetic (EPR) and nuclear magnetic resonance (NMR) – experiments. In particular, degradation under ‘fast charging’ conditions, i.e. Lithium plating and dendrite growth, can be studied in real time.

Understanding structure and functionality of interfaces is also key to solid-state bat-

teries. These are used either as thin-film cells in integrated devices for applications in microelectronics or as ceramic thick-film cells with potentially improved volumetric energy density and high safety for automobile applications.

Both concepts have in common requirements as high cycling performance, high thermal stability, high capacity and high rate capability. The main objective of current research is to overcome interface issues related to poor mechanical contact and limited electrochemical stability. A monolithic concept is outlined by combining electroactive phosphate materials with adapted microstructures. Based on several combinations of materials, three

phosphate compounds were synthesized and used as electrolyte and electrode materials, respectively. Accordingly, an all-phosphate solid-state lithium-ion battery was developed that allows high cycling performance of several hundredths cycles, as well as high rate capability.

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Fri, 9:35 a.m.

ULTRAFAST SPECTROSCOPY OF CHARGE AND STRUCTURAL DYNAMICS IN HYBRID PEROVSKITES

Felix Deschler

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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.

Fri, 10:05 a.m.

FIRST-PRINCIPLES STUDIES OF RADIATIVE AND NONRADIATIVE RECOMBINATION IN HALIDE PEROVSKITES

Chris G. Van de Valle

Materials Department, University of California, Santa Barbara, California, USA

Understanding the origin of the high solar conversion efficiency of halide perovskites is of key importance to the field. We explicitly compute radiative and nonradiative in the prototypical hybrid perovskite, $(\text{CH}_3\text{NH}_3)\text{PbI}_3$, as well as in other halide perovskites.

I will first briefly discuss the methodology that allows us to calculate recombination coefficients completely from first principles. Some research groups attributed the high efficiency to low radiative recombination due to strong Rashba spin-orbit coupling. We demonstrate that the radiative recombination in hybrid perovskites is actually strong, and that spin-orbit coupling has only a minor impact on radiative recombination [1,2]. The computed radia-

tive recombination coefficient is as high as in typical direct-gap semiconductors used in optoelectronics.

The demonstrated high radiative recombination coefficient thus enables promising applications in light-emitting diodes. However, our first-principles calculations of nonradiative rates show that strong Auger recombination will suppress efficiency [3]. Fortunately, our insights into the origins of the strong Auger recombination indicate potential avenues for engineering the Auger coefficient. Finally, I will discuss defect-assisted recombination, which is a limiting factor for both light emitters and solar cells, and is closely coupled to the issue of degradation.

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Poster Sessions

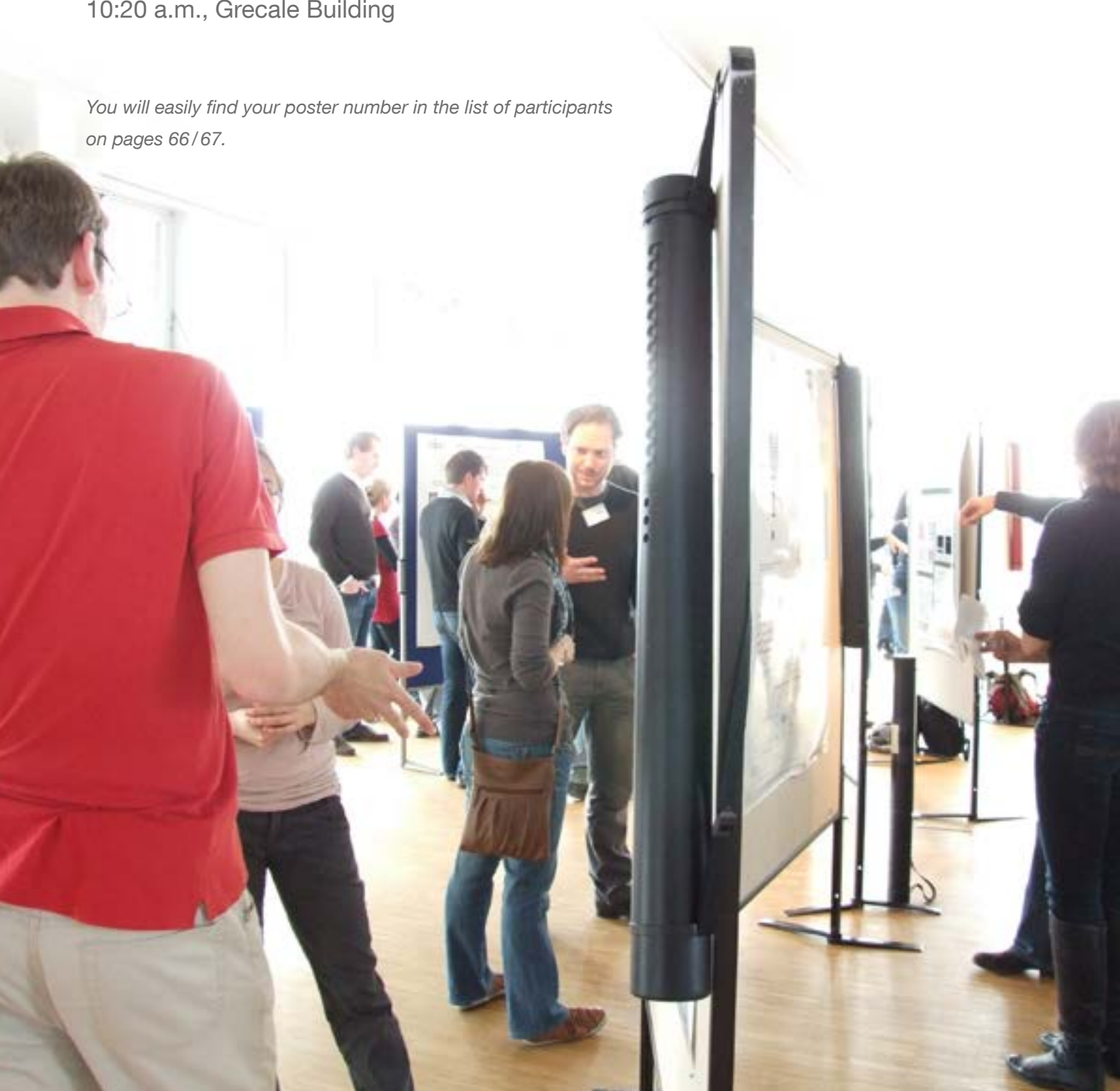
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HELICAL POLYMERS AND THEIR CHARGE TRANSPORT PROPERTIES

Mahshid Alizadeh, I. Huc

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The synthetic foldamers, or oligomers that fold into stable conformations in solution, mimic the well-defined conformations, such as helices and β -sheets, of proteins and nucleic acids [1]. These organic materials have been utilized in a wide range of contexts including surface recognition, encapsulation of guest molecules such as saccharides, charge transport, catalysis. In addition, their semiconducting properties make them candidates for the bottom-up fabrication of electronic circuits incorporating them as organic compounds. Up to now, some attempts to synthesize high length helices have been successful, but these synthetic pathways are labour intensive and not easily adapted to a large-scale production [2-3].

Three approaches have been developed to synthesize foldamers: (i) the step-by-step growth by repetitive addition of a monomer, or more extended units, to a growing chain. This approach works well on solid support. (ii) Convergent, e.g. segment doubling, iterative approaches which allow more rapid chain lengthening. (iii) Polymeric growth as a rapid chain growth represents the third approach.

This project explores a new polymerization approach to the synthesis of the high length well-defined aromatic helices within Metal-organic framework (MOF) or to be used in organic monolayers exploiting their remarkable charge transport properties. The research plan will involve three sequential parts: 1) preliminary fundamen-

tal investigations on the synthesis of the desired monomers, 2) tuning of the polymerization method to synthesize the high length helices, 3) investigation of charge transport properties of the obtained high length helices.

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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 to 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 interests, closing the gap of our measurements between tetragonal and orthorhombic phase. As a result of our more detailed spectroscopic and microscopic measurement techniques, we want to show the local behavior of single crystals within the thin films during the phase transition.

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The transport of H adatoms across oxide supports plays an important role in many catalytic reactions. We investigate the dynamics of H/Fe₃O₄(001) between 295 and 382 K. Using fast scanning tunneling microscopy (FastSTM) [1,2] at frame rates of up to 19.6 fps, we observe the thermally activated switching of H between two O atoms on neighboring Fe rows.

Importantly, our local measurements show that the activation barrier and thus switching rate of individual species varies significantly with their local chemical environment, i.e. in proximity to a defect. Density functional theory explains this phenomenon as a defect-induced distortion in the

Fe–O lattice which shortens the length of the diffusion path. Quantitative analysis yields an apparent activation barrier of 0.94 ± 0.07 eV on a pristine surface.

We determined that the experimentally obtained activation barrier results purely from energetics and does not contain any entropic contributions to the Gibbs free energy. Furthermore, we do not observe any long-range diffusion of hydrogen up to approximately 450 K, at which point hydrogen is known to desorb from the surface [3,4]. The present work highlights the importance of local techniques such as STM in the study of atomic-scale dynamics at defective surfaces such as oxide supports.

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PASSIVATION OF DEFECTS WITH ORGANIC AMMONIUM SALTS FOR EFFICIENT AND STABLE MAPbI₃ PEROVSKITE SOLAR CELLS

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The high efficiency as well as the easy solution and low temperature processability of perovskite films keeps it ahead of the game among photovoltaic technologies. However, the polycrystalline property of low temperature solution processed perovskite film inevitably leads to the presence of crystallographic defects at perovskite surfaces and grain boundaries (GBs) [1]. For example, the methylammonium ion (MA⁺) in MAPbI₃, a volatile organic cation, under the high heat and/or moisture -ever present environmental conditions- can be easily released from the 3D lattice [2].

This releasing of MA⁺ further causes the generation of different types of defect such as under-coordinated Pb and Pb-I antisite defects [3]. These defects adversely 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 (MAPbI₃) and hole transporting layer to passivate these inevitable defects at GBs and surface to obtain more stable and higher efficient solar cells. After treatment, over 10 % PCE enhancement is observed compared to the reference, mainly due to the improved V_{oc} and FF. Achieved results support us in the artful molecular design of new passivators to make perovskite solar cells more promising and reliable for industrial applications.

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Photosystem I (PSI) is a remarkable multiprotein complex in plants and cyanobacteria which catalyzes light-driven charge separation to generate universal cellular reductive equivalents. Despite being composed of 11-14 protein subunits and around 100 (mostly pigment) cofactors [1], isolated PSI is extraordinarily durable and accessible to a variety of alternative electron donors and acceptors; these include proteins, small organic compounds, as well as 2D/3D electrode scaffolds such as graphene, modified gold [2] or antimony-doped tin oxide [3].

The latter allow for incorporation of PSI into bio-hybrid photovoltaic devices in order to exploit its great quantum efficiency (~0.95 [4,5]) for photocurrent generation. Moreover, such defined systems could assist in elucidating energy transfer processes

within the PSI reaction center, and to unravel potential target sites for improvement by protein engineering.

Generating suitable PSI variants requires a workhorse organism that is (i) productive and (ii) easily genetically modifiable. Both criteria are met by *Synechocystis* sp. PCC6803, a single-celled cyanobacterium with extremely high PSI abundance as compared to plants, and a genome readily accessible to editing through homologous recombination. Scar-less gene editing without disturbing gene functionality at any given time point has been established in our lab, allowing us to customize the genetic blueprint of PSI in vivo to finally assemble large quantities of variant PSI for bio-hybrid characterization and application.

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Semiconductor nanowires (NW) with low band gap have become widely studied nanostructures for advanced nanoelectronics, mid-infrared optoelectronics, as well as photo-conversion applications. In particular, advanced concept NW solar cells attempt to exploit strong quantum confinement effects, which requires to access ultrascaled geometrical regimes of very small NW diameters. For example, in low-gap InAs NWs very strong and tunable quantum confinement effects are expected to occur for diameters well below 30 nm [1,2] – which has hitherto been difficult to reach.

Here, we present InAs NWs grown along the [111] direction on SiO₂-masked Si(111) using a completely catalyst-free vapour-solid (VS) growth mechanism [3,4] via

selective-area molecular beam epitaxy. In a first approach we show how by direct bottom-up epitaxy the NW dimensions can be controlled by tuning the growth parameters to finally obtain sub-25 nm diameter InAs NWs. In a second approach, we explore a so-called reverse reaction growth mechanism to intentionally thin as-grown NWs by in situ thermal annealing [1,4]. Starting from > 1.5 µm long NWs with diameters of > 90 nm we performed various different thermal annealing experiments by varying in situ vacuum conditions, As-overpressure, annealing temperature and time. We thereby realized microstructure conserving InAs NWs (resolved by TEM analysis) with diameters < 15 nm [4]. First preliminary low-temperature PL spectra of a NW-array with sub-30 nm diameter show a complex scaling behaviour of the energy

emission with diameter, which is attributed to a competition between band-to-band luminescence and indirect transitions due to surface states and stacking defects.

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Efficient electrocatalysis has a prominent role in solving the recent energy related challenges. A fundamental understanding of the processes at the electrified interfaces is of crucial importance for increasing their efficiency. Herein, we present the laser induced current transient (LICT) technique as a new methodology for studying the electrode/electrolyte interface processes.

The LICT technique utilizes the so-called temperature jump effect. The sudden heating of the electrode surface leads to a short change of the orientation of interfacial water. The response of the system can be recorded as current transient which corresponds to the sign of the excess electrode surface charge [1]. The potential of maximum entropy (PME), at which the current transient changes the sign, can be identified [2]. When composition and structure of the electrode surface are fixed, the reaction is likely to be faster when the equilibrium potential of

this reaction is close to the PME, at which the electric double layer reaches maximal “disorder” and energy barrier for electron transfer is lowest.

We present the results of the LICT technique on how pH of electrolyte influences the PME and electrocatalytic activity. Two electrocatalytic reactions, hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), are performed on polycrystalline Pt and Au electrodes in different pHs. The obtained results reveal the PME moves further away from the thermodynamic equilibrium potential of the HER (0.00 V vs RHE), but closer to the corresponding value of the ORR (1.23 V vs RHE) with pH increase, which results in the increase of the ORR activity [3]. Additionally, the same PME measurement but with O₂ saturation has been performed and we found the PME values are more positive than in Ar saturated electrolytes. This is because the protons are consumed by dissolved O₂, which leads to a change of

the local pH at the interface between electrode and electrolyte [4]. All the obtained data emphasize the role of the electrolyte composition for the kinetics and mechanisms of the interfacial processes.

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IMPACT OF SURFACE ADSORBATES ON CHARGE CARRIER TRANSPORT IN METAL-OXIDES FOR SOLAR WATER SPLITTING

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Photoelectrochemical (PEC) water splitting is a promising route for efficient conversion of solar energy to chemical fuels. Among different photoelectrode materials, bismuth vanadate (BiVO₄) is one of the most actively investigated oxide semiconductors. Here, we employ photoconductive atomic force microscopy (AFM) under controlled *in-situ* conditions to gain insight into the relationship between surface interactions and interfacial charge transport characteristics in polycrystalline BiVO₄ thin films. We demonstrate that the low intrinsic bulk conductivity of BiVO₄ limits charge transport through the film, and

that the transport mechanism can be attributed to space charge limited current in the presence of trap states [1].

By analyzing the space charge limited current in selective gas environments, we are able to quantify the impact of surface adsorbates on bulk transport properties. We find that surface adsorbed oxygen acts as a shallow trap state and accounts for 40 % of the effective trap density in BiVO₄ thin films [2].

Understanding such limitations of charge transport and transfer in PEC photoelec-

trodes at the nanoscale and under *in-situ* conditions will enable the design of next generation PEC materials.

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Harvesting solar energy by converting abundant chemicals photocatalytically into valuable products is still far from being practically applied on a large scale. Aspirant applications are the production of hydrogen by water splitting, biomass reforming or the fixation and valorization of greenhouse gases such as carbon dioxide and methane [1,2,3]. Investigations of model catalysts under ideal conditions, such as single crystals in ultrahigh vacuum, give essential insights into fundamental photocatalytic processes. Yet, drawn conclusions cannot always be readily transferred to environmental conditions due to a phenomenon known as “pressure gap”. On the other hand, reactions on a macroscopic scale are usually carried out

at ambient conditions, but require large amounts of catalytically active material. Therefore, one challenge is the transfer of the chemistry observed for the model systems studied in *e*-conversion and obtained under UHV to ambient systems.

A further one is that new photocatalysts developed by several PIs of *e*-conversion are often only available in low amounts due to sophisticated synthesis methods. In both cases a limited catalyst loading requires the determination of catalytic properties with a highly sensitive device to identify and quantify reaction products [4]. Herein, we discuss different setups allowing the evaluation of activity, selectivity and stability of heterogeneous photocata-

lysts at ambient conditions for relevant reactions, facilitating the comparability of the samples within the scope of the *e*-conversion cluster.

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AMMONOTHERMAL SYNTHESIS OF TERNARY GRIMM-SOMMERFELD ANALOGOUS NITRIDE SEMICONDUCTORS II-IV-N₂ (II = Mg, Mn, Zn; IV = Si, Ge)

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Due to the wide field of possible applications (e.g. photovoltaics, solid-state lighting) and the rapidly growing market, the research into efficient optoelectronic semiconductor materials is crucial to meet the high requirements of modern electronic technologies. Currently, group 13 nitrides and their solid solutions (Al,Ga,In)N are the most frequently used materials [1]. However, Ga and In are scarce elements, which requires their replacement with more earth-abundant materials. Therefore, especially ternary Grimm-Sommerfeld

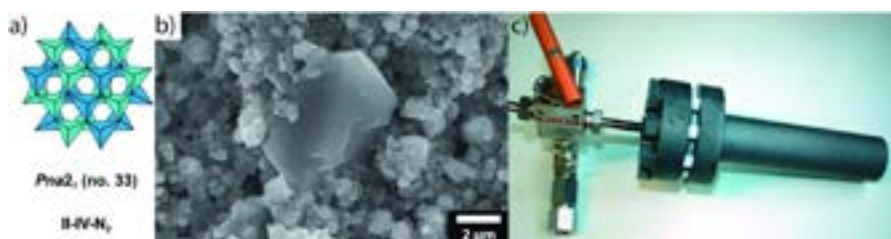
analogous II-IV-N₂ (II = Mg, Mn, Zn; IV = Si, Ge, Sn) have attracted great interest, as they are structurally related to group 13 nitrides (Figure 1a) and exhibit similar electronic and optical properties [2].

Recently, we succeeded in the ammonothermal synthesis of these II-IV-N₂ semiconductors as well as solid solutions of them by using supercritical ammonia as solvent (Figure 1b) [3,4]. To generate the required reaction conditions ($T \geq 870$ K, $p \geq 150$ MPa), custom-built high-pressure,

high-temperature autoclaves made of nickel-based superalloys were constructed (Figure 1c). The spectroscopic characterisation of the Grimm-Sommerfeld analogous nitrides showed, that a wide range of bandgaps (2.5 – 4.8 eV) can be attained. Therefore, the ammonothermal synthesis has proven to be a promising method for the development of next-generation semiconductor materials.

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Wurtzite-type superstructure of II-IV-N₂ nitrides (a). SEM image of ZnSiN₂ crystals (b). Autoclave made of nickel-based superalloy with flange construction for explorative ammonothermal syntheses (c).

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Electrocatalytic hydrogenation is a promising, sustainable technology for the ambient reduction of organic molecules. The required hydrogen is produced *in situ* from electrolysis of water or reduction of hydronium ions, which is driven by renewable resources [1]. The *in situ* adsorption and formation of hydrogen on the electrode surface are two crucial steps in electrocatalytic hydrogenation of organic compounds. In acid solution, it is believed that these occur either via a *Volmer Heyrovsky* or a *Volmer-Tafel* sequence [2].

Considering that pH changes the open circuit potential on Pt, we evaluate in this work how the binding strength of H on Pt depends on the electric potential applied to Pt. The H binding energy is determined on carbon nanotube supported platinum (Pt/CNT), using a kinetic method measuring the HD and D₂ formation rates in the reaction of D₂ with liquid D₂O [4]. It is shown that the desorption barrier of H from Pt is constant with pH, whereas its adsorption barrier increases with decreasing pH, thus giving a lower binding energy at lower pH.

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It is known that a lower pH will promote both the reaction rates of hydrogen evolution and electrocatalytic hydrogenation. This is reported to be a consequence of a weaker hydrogen binding with the Pt surface, making it more reactive. However, the driving force for the weak binding of H on Pt at low pH is still unclear, hindering the rational design of more efficient catalysts [3].

Lower pH, meaning a higher concentration of hydronium ions at the Pt surface, will induce more compact electric double layers, which is hypothesized to impede the adsorption of H. This will also be supported by measuring the adsorption/desorption barrier of H under an externally added potential on Pt.

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ADVANCED THERMOELECTRICS IN HIGH-MOBILITY GaAs-ALGaAs CORE-SHELL NANOWIRES

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Semiconductor nanowires (NW) are promising one-dimensional (1D) systems for thermoelectric energy conversion applications. A particularly appealing feature of 1D-NWs is that electrical and thermal effects can be theoretically decoupled. By working in the ballistic transport regime, high electrical conductivity, large Seebeck coefficients and enhanced thermopower may thus be achieved. However, the simultaneous realization of low thermal conductivity is a challenge, since the large surface-to-volume ratio responsible for high phonon scattering also usually increases electron scattering thus preventing ballistic 1D transport. This encourages the development of completely new approaches for designing efficient nanowire thermoelectrics and a novel platform is

presented in this work.

Our studies are based on high-mobility Si-delta doped GaAs/AlGaAs core-shell NW heterostructures, which hold the potential for both high-performance steep-slope NW-field effect transistors (NW-FET) [1] and for in-depth investigations of low-temperature quantum transport [2]. Top-gated NW-FETs were used to study the quantum transport characteristics at low temperature (4-7 K). During pinch-off we observe clear plateau-like signatures, consistent with the depopulation of quasi-1D subbands as confirmed by correlated simulations [2]. Subsequent Seebeck effect measurements show distinct quantum oscillations in the Seebeck voltage as a function of applied gate voltage and dif-

ferent heater powers which correspond to the 1D-like plateaus in conductivity [3]. Furthermore, thermal conductivity measurements at room temperature were carried out on suspended NWs using Raman spectroscopy, which yield a significant reduction to values as low as $3 \text{ Wm}^{-1}\text{K}^{-1}$ [3].

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SHORT-RANGE CORRELATED DISORDER AND URBACH ENERGIES IN HALIDE PEROVSKITES

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Halide perovskites (HaPs) are intriguing optoelectronic materials and promising candidates for efficient solar-cell devices. They allow for efficient collection of sunlight in thin-film photovoltaic devices due to advantageous physical properties, such as small Urbach energies and sharp optical absorption edges. Notwithstanding, they differ from usual efficient optoelectronic materials by their complex nuclear dynamics and structural effects, including anharmonicity and disorder. This is particularly interesting since small Urbach energies indicate a low amount of disorder.

To shed light on these seemingly contradicting features of HaPs we study the disorder potential induced for electronic states in three HaP compounds by density functional theory (DFT) and DFT-based molecular dynamics simulations [1]. This

approach intrinsically incorporates finite temperature effects in the nuclear dynamics including anharmonicity to all orders in the Taylor expansion of the crystal potential. We find that correlations in the disorder potential are dynamically confined to atomic distances. These short-range correlations are a consequence of the nuclear motions of A-site and X-site ions which dynamically shorten the disorder.

As a result, the correlations in the disorder potential show similar length-scales as the ones known for usual inorganic semiconductors leading to favorable distributions of band-edge energies. We conclude that sharp optical absorption edges and small Urbach energies, which are highly desired properties of solar absorber materials, are enabled by the dynamical shortening of correlations in the disorder potential.

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The presence of lead in novel hybrid perovskite-based solar cells remains a significant issue regarding commercial applications. Therefore, antimony-based perovskite-like $A_3M_2X_9$ structures are promising new candidates for low toxicity photovoltaic applications. So far, methylammonium antimony iodide ($MA_3Sb_2I_9$) compounds display the highest solar cell efficiencies if crystallized in a 2D layered structure. In this layered phase, the compound benefits from a direct and narrow bandgap.

However, the formation of $MA_3Sb_2I_9$ in the undesired 0D dimer phase with an indirect bandgap is more thermodynamically favorable. So far, only the incorporation of chloride into the structure enabled the suppression of the dimer phase in $MA_3S_2I_9$ and resulted in thin films with direct bandgaps of around 2.17 eV.

Here, we demonstrate a new fully alcohol-based synthesis procedure for pure iodide-based compounds in the 2D phase with a bandgap below 2 eV and high-quality mor-

phologies, resulting in efficient solar cells. Moreover, using *in situ* XRD methods, we report on the stability of the layered phase towards moisture and high temperature. Our work shows that careful control of nucleation via processing conditions can provide access to promising perovskite-like phases for photovoltaic applications.

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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 ranging from the renewable generation of fuels from sunlight to advanced quantum emitters [1].

Especially monolayer transition metal dichalcogenides (TMDs) in the form of MX_2 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 MoS_2 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. These materials will be integrated into photoelectrochemical cells and configured as gate tunable working electrodes in a four terminal field effect transistor (FET) configuration. Using such 2D heterostructures, we seek to achieve nanoscale charge separation using interlayer excitons and control energy band positions and carrier concentrations by gating the 2D heterostructure.

The goal of this work is to investigate coupled charge injection and chemical mechanisms at the solid 2D heterostructure/liquid interface and, ultimately, to realize selective (photo)electrochemical reactions by affecting catalytic overpotentials.

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TRACKING THE IMPACT OF TERNARY SENSITIZATION ON THE 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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DO DIFFERENT DEVICE ARCHITECTURES OF PEROVSKITE SOLAR CELLS HAVE DIFFERENT DEGRADATION MECHANISMS?

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The global energy demand increases significantly with the ever-increasing population, combined with industrialization and development. Fossil fuels are non-sustainable sources of energy and using fossil fuels results in global warming. Assuming a 20 % efficiency of solar cells receiving 1000 W/m² for 8 hours a day, the global energy consumption can be easily satisfied with just under 500,000 km² of solar panels based on currently available technologies easily. However, solar energy is still not widely adopted because of the higher cost per unit of electricity generated from solar panels. One of the main reasons for this is the high initial costs involved in fabricating ultra-pure silicon, which makes up most commercially available solar cells reaching up to efficiencies of above 20 %. For this reason, the different technologies of next generation thin film solar cells have emerged during last years. Several different technologies have emerged. Among these new technologies, 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 researches on PSCs are performed by a simple current-voltage measurement. Therefore, it is necessary to introduce new characterization tools for analyzing degradation mechanisms of PSCs.

We investigate degradation processes of different device architectures of PSCs under illumination condition with *in situ* grazing

incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small angle 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 degradation mechanisms for different device architectures, potential solutions could be found to suppress the degradation.

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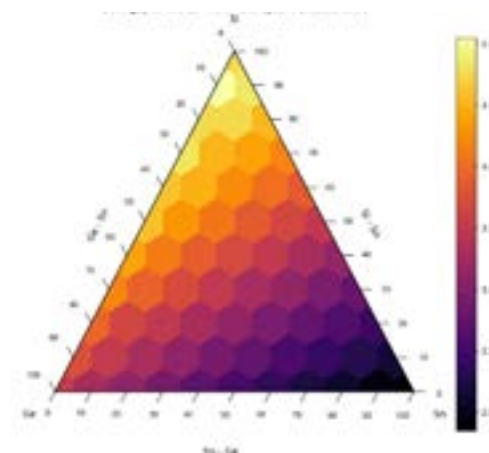
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The semiconductor compounds Zn-SnN_2 , ZnGeN_2 and ZnSiN_2 are promising new materials to be used for example as photovoltaic materials. A crucial material property for such applications is the band gap that is usually found to be too small from standard density functional theory (DFT) band structure calculations.

As our results demonstrate, this problem can be solved by using the so-called modified Becke-Johnson or Tran-Blaha functional [1] that leads to band gaps in very good agreement with experiment. The gap in the aforementioned materials can be continuously varied and this way optimized by alloying on a sublattice, as for example $\text{Zn}(\text{Sn,Ge})\text{N}$ with a more or less random occupation on the Sn-Ge sublattice. Use of the CPA (Coherent Potential Approximation) alloy theory [2] allows to describe such disordered non-stoichiometric systems without the use

of the expensive super cell technique.

Corresponding results based on the first common implementation of the Tran-Blaha-functional and the CPA for disordered alloys will be presented for all possible binary combinations as well as for the so far unexplored system $\text{Zn}(\text{Sn,Ge,Si})\text{N}_2$ (see figure). These results will complement corresponding experimental work of the group of Prof. W. Schnick and coworkers. In addition to the determination of the gap as a function of composition, X-ray spectra are calculated for the K-edge of N to supplement the experimental determination of the gap.



Band gap for the semiconductor system $\text{Zn}(\text{Ge,Sn,Si})\text{N}$

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An in-depth, atomic-level characterization of solid-liquid interfaces is crucial for the design of a wide range of energy conversion systems such as electrocatalysts, batteries or fuel cells. Predictive-quality quantum mechanical (QM) simulations can make most valuable contributions to this end, but are challenged by the treatment of the liquid environment – even when relying on computationally most efficient approaches like semi-local density-functional theory (DFT).

Traditionally, the electrochemical stability and activity at such interfaces has therefore been analyzed from charge-neutral DFT calculations, often considering only a very reduced set of interfacial degrees of freedom, e.g. only adsorbates that are

chemically bound to the electrode surface. Recently, it has been shown that an inclusion of mean-field solvation and electrolyte effects via hybrid QM/continuum models allows to determine electrochemical properties with much better accuracy and at only marginally higher computational costs [1,2].

We will present recent developments in simulation strategies of electrochemical interfaces within such implicit solvation schemes, using the ENVIRON [3] module of Quantum ESPRESSO, and assess its accuracy by comparison to experimental and theoretical results.

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IN-SITU VISUALIZATION OF HYDROGEN EVOLUTION SITES ON HELIUM ION TREATED MOLYBDENUM DICHALCOGENIDES UNDER REACTION CONDITIONS

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Nanostructured 2D transition metal dichalcogenides play an increasingly important role in heterogeneous catalysis. The materials are abundant and cost effective (co-)catalysts with tunable physical properties to catalyze a number of key reactions related to energy provision, for instance hydrogen evolution reaction (HER) or carbon dioxide reduction. It is vital to understand which surface sites are highly active in order to maximize their number and to improve the overall (photo-)catalytic behavior of those materials.

Here, we visualize in-situ the catalytically active sites at the surface of mechanically exfoliated molybdenum dichalcogenides (MoX₂, X = Se, S) with lateral resolution on

the nanometer scale by means of electrochemical scanning tunneling microscopy. The edges of single MoX₂ flakes show high catalytic activity, whereas their surfaces are inactive. We demonstrate how the inert basal plane of these materials can be activated towards the HER with the help of a focused beam of a helium ion microscope. Our in-situ visualization allows to demonstrate that the helium ion induced basal plane defects contribute at lower potentials to the HER than the edges, while the activity of the edges exceeds the activity of the basal defects for sufficiently high potentials.

Given the lithographic resolution of the helium ion microscope, our results show the

possibility to generate active sites in transition metal dichalcogenides with a spatial resolution below a few nanometers.

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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]. On the other hand its wide band gap only allows harvesting of the small UV portion of the solar spectrum which strongly limits its efficiency for solar energy conversion. Thermal treatment of TiO_2 films induces the formation of sub-bandgap oxygen vacancies states (OV-TiO_2), enabling visible light absorption into the substoichiometric material [2].

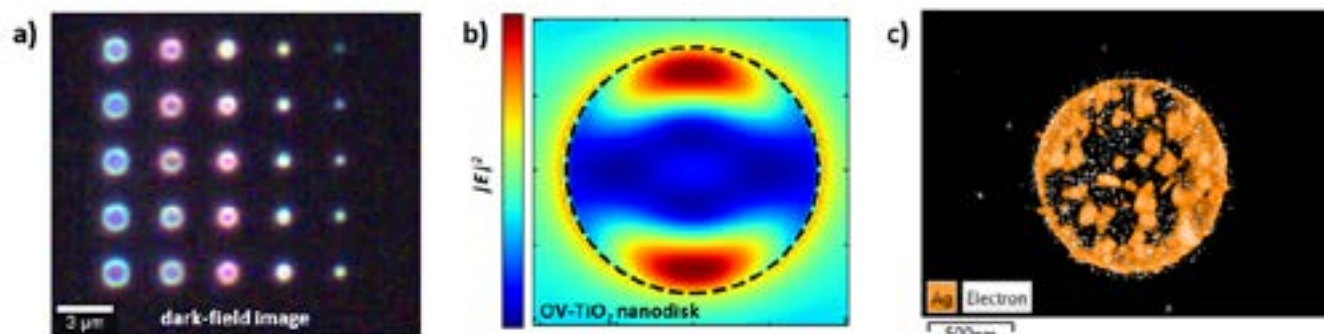
In this work we shape OV-TiO_2 into nano-disks (Fig. a) exhibiting anapole resonances in the visible [3,4]. This mode is characterized by the annihilation of its far-field scattering due to destructive electric and toroidal dipole interference, providing a maximum of electric energy inside the

resonator (Fig. b). The goal of this work is to 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 532 nm laser excitation at a single particle level (Fig.c). As a continuation we investigate to which extend the anapole-driven absorption enhancement can be transferred to other materials with photocatalytic potential.

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SITE-SELECTIVELY GENERATED PHOTON EMITTERS IN MONOLAYER MoS_2

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We demonstrate the site-selective generation of single defect emitters in a monolayer MoS_2 van der Waals heterostructure [1]. We irradiate monolayer MoS_2 with helium ions to generate optically active defect luminescence [2] and encapsulate the defective MoS_2 within hBN to greatly enhance optical quality [3]. The encapsulation of the defective MoS_2 reveals narrow spatially localized spectral lines that exhibit emission that is redshifted by 100 - 200 meV below the neutral 2D exciton.

We spectroscopically investigate single emitters by performing photoluminescence excitation spectroscopy and temperature dependent measurements. The

line shape reveals a strong asymmetry resembling the interaction with LA/TA phonons. Employing the independent Boson model to our emission lines, we find that the emitters are spatially localized to a length scale of 2 nm. Moreover, irradiation through a fully hBN encapsulated monolayer MoS_2 results in highly homogeneous defect emission [4]. We attribute the emission to atomistic defects induced by the helium ion irradiation and discuss their origin in the light of scanning tunneling microscopy measurements [5]. Our work paves the way towards the controlled and deterministic generation of single quantum emitters in monolayer TMDC van der Waals heterostructures.

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DISCRETE INTERACTIONS BETWEEN TRAPPED INTERLAYER EXCITONS AT A MoSe_2 - WSe_2 HETEROINTERFACE

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Interlayer excitons (IXs) in hetero-bilayers of transition metal dichalcogenides [1] have remarkable properties that open up tantalizing prospects of Bose-Einstein condensation [2], excitonic superfluidity at elevated temperatures [3] and novel quantum phases, such as Wigner crystallization at low temperatures [4]. Here, we trap a tunable number of IXs within a nanoscale confinement potential induced by placing a MoSe_2 - WSe_2 hetero-bilayer onto an array of nanopillars. We control the mean occupation of the trap via the optical excitation level, identify different localized IX states via their sharp-line emission and characteristic power dependencies and directly measure the hierarchy of dipolar IX-IX interactions. Emission from the interlayer biexciton, triexciton and quadexciton

is found to be blue-shifted from the single exciton by (8.4 ± 0.6) meV, (12.3 ± 0.5) meV and (16.8 ± 0.3) meV, respectively.

We reproduce this energy spectrum by modelling the repulsive dipole-dipole interactions of maximally spaced excitons in a harmonic trapping potential. Furthermore, all multi-excitonic emission lines split into doublets. We calculate the exchange energy for the biexciton in a configuration-space approach [5] and match the observed splitting of (1.2 ± 0.5) meV for realistic material parameters and a confinement length of 3 nm. Our results demonstrate probing of dipolar interactions at the few-exciton limit, potentially opening a route to explore emergent quantum phases.

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InGaAs nanowire (NW) arrays have emerged as important active materials in future photo-voltaic and photodetector applications, due to their excellent electronic properties and tunable band gap [1,2].

Here, we report a systematic investigation of the optical absorption characteristics of composition-tunable vertical InGaAs nanowire (NW) arrays. Using finite-difference time-domain simulations we first study the effect of variable composition (Ga-molar fraction) and NW array geometry (NW diameter, period, fill factor) on the optical generation rate. NWs with typical diameters in the range of ~100-250 nm lead to generation rates higher than the equivalent bulk case for moderate fill factors (NW period of ~0.3-0.8 μm), while slightly smaller fill factors and increased

diameters are required to maintain high generation rates at increased Ga-molar fraction [3].

The optical absorption was further measured using spectrally resolved ultra-violet-visible-near-infrared (UV-Vis-NIR) spectroscopy on NW-arrays transferred to transparent substrates. Interestingly, large variations in Ga-molar fraction ($0 < x(\text{Ga}) < 0.5$) have a negligible influence, while minute changes in NW diameter of less than $\pm 20 \text{ nm}$ affect the absorption spectra very strongly, leading to pronounced shifts in the peak absorption energies by more than ~700 meV [3]. These results clearly highlight the much larger sensitivity of the optical absorption behavior to geometric parameters rather than to variations in the electronic band gap of the underlying NW array.

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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 spec-

troscopy, 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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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} Scm^{-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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ACCURATE AND EFFICIENT WAVEFUNCTION BASED COMPUTATIONAL PROTOCOLS CAPABLE OF EXPLORING ENERGETICS AND SPECTROSCOPIC PROPERTIES OF SOLIDS AND SURFACES

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Developing the information content of catalytically active intermediates in heterogeneous catalysis is a difficult problem. Partially this is due to the lack of reliable theoretical tools that are able to compute energetics and simulate spectra with predictive accuracy that can lead to meaningful structural correlations.

Ab initio wave function based reference calculations were, until recently, either not tractable for the large system sizes imposed by surface problems or too demanding to be applied routinely. The se-

vere limitations imposed by the steep scaling of the wave function based methods with system size can be overcome by exploiting the relative short-range character of the dynamical correlation through the concept of local correlation techniques.

Similarly, for non-metallic systems the system size that needs to be treated quantum mechanically can be effectively reduced by employing embedded cluster models that treat the long-range electrostatics and polarization on a molecular mechanical level.

In this contribution it will be shown that by describing the quantum region at the level of the Domain-based Local Pair Natural Orbital CCSD(T) approach (DLPNO-CCSD(T)) [1,2] the adsorption energies for a set of small molecules at the rutile $\text{TiO}_2(110)$ surface can be computed with errors of $< 0.04 \text{ eV}$ with respect to the available experimental values [3].

Likewise, by describing the quantum region at the level of the Similarity Transformed Equation of Motion Coupled-Cluster (bt-PNOSTEOM-CCSD) [4,5] the

optical band gaps of a study set of organic and inorganic semiconductors can be computed with errors that are on average lower than 0.2 eV with the available experimental values [6].

Hence the above computational protocols contain strong predictive accuracy that is able to provide access to the reaction energetics and the spectroscopic properties of complicated reaction mechanisms. A case study is discussed for the water splitting reaction on rutile $\text{TiO}_2(110)$ surface.

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TUNING SELECTIVITY OF ELECTROCHEMICAL CO_2 REDUCTION AND HYDROGEN EVOLUTION REACTION ON METAL MODIFIED SILICON/SILICON-OXIDE ELECTRODES VIA BICATALYTIC MECHANISMS

28

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Producing fuels from CO_2 and sunlight is one of the key technologies for the future of our energy economy. In order to achieve an efficient conversion, the catalyst has to meet several requirements, such as stability, selectivity towards the desired product and an appropriate lowering of the kinetic barrier. In order to minimize kinetic overpotentials and to tune selectivity of metal based catalysts for the CO_2 reduction reaction (CRR) and the hydrogen evolution reaction (HER), we present two types of mesoscopically structured electrodes exhibiting enhanced reactivity that we attributed to a bicatalytic mechanism: (1) metal islands on oxide-silicon electrodes as well as (2) bimetallic Cu/Au structures.

Recent studies conducted in our group showed that the selectivity of the CRR/HER on silicon/silicon oxide electrodes covered with gold nanostructures, which are fabricated by nanoimprint lithography [1], depends on geometric properties [2]. The observed increase of the HER rate with decreasing structure size of gold islands indicates a bicatalytic mechanism taking place on the metal/oxide phase boundary.

The second approach is based on a study of copper electrodes covered with gold nanoparticles by the group of Jaramillo [3]. The authors found increased selectivity towards products containing C-C bonds (such as ethylene) at low overpotentials and explained this observation by complementary chemical reactions taking place on both metals in close proximity [3].

We aim to take advantage of this tandem catalytic effect by using inter-digital-array electrodes with both a gold and a copper comb-like structure, which can be addressed individually. This tandem electrode allows for investigation of the product distribution of the CRR at different CO formation rates at the Au and different overpotentials at the Cu electrode.

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CONTROLLING MULTI-PHOTON ABSORPTION EFFICIENCY BY CHROMOPHORE PACKING IN METAL-ORGANIC FRAMEWORKS

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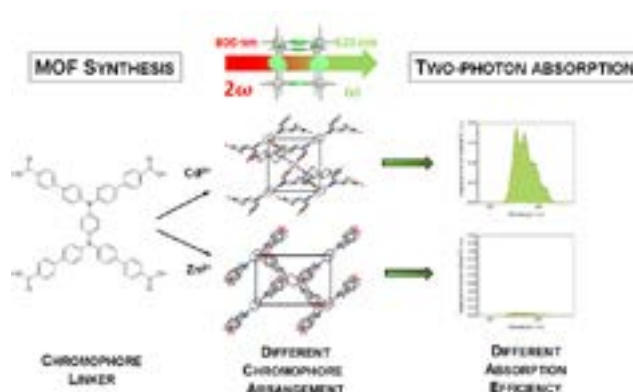
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Coordination polymers show great potential for the tailored design of advanced photonic applications by employing crystal chemistry concepts [1]. One challenge for achieving a rational design of non-linear optical active MOF materials is deriving fundamental structure-property relations of the interplay between the photonic properties and the spatial arrangements of optically active chromophores within the network.

We here investigate two-photon absorption (TPA) induced photoluminescence of two new MOFs based on a donor-acceptor tetraphenyl-phenylene diamine (tPPD) chromophore-linker (H_4 TPBD) and Zn(II) and Cd(II) as metal-centers. The TPA efficiencies are controlled by the network topologies, degree of interpenetration, packing densities and by the specific spa-

tial arrangement of the chromophores. The effects can be rationalized within the frame of established excited-state theories of molecular crystals [2]. The results presented here demonstrate the key impact of chromophore orientation on the non-linear optical properties of crystalline network compounds and allow for establishing quantitative design principles for efficient TPA materials.



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SILVER-COATED GOLD NANORODS ON DNA ORIGAMI

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DNA origami allows for the organization of nanoparticles in a controlled manner which has become an important tool for manipulating light at the nanoscale, e.g. in photonics and electronics [1]. Yet, the strategy has been applied to a limited number of different plasmonic nanoparticles (e.g. gold nanospheres and -rods (AuNS and AuNRs), silver spheres (AgNS)). The optical behavior of cooperative bimetallic nanoparticles has remained virtually unstudied.

Here, Au/Ag core-shell NRs were conjugated with DNA origami for the purpose of exploring and tuning synergistic effects such as chirality as well as plasmonic phenomena in ordered metal nanoparticle

systems. Silver is known to exhibit a long plasmonic lifetime, sharp resonance band, and a large plasmon tunability range and thus displays superior plasmonic properties compared to gold [2]. The silver coating of AuNRs results in an enhancement of plasmonic properties displayed in higher circular dichroism and absorption signals as compared to pristine AuNRs [3].

Arranging bimetallic nanoparticles on DNA origami allows us to create and gain deeper insights into physical phenomena of these new optical systems. Eventually, this should drive progress in plasmonic and other light-guiding applications.

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Improving the performance of third generation photovoltaic materials requires a broad knowledge of their molecular behaviour. In organic solar cells, as well as in perovskite systems, polarons are the main charge carrier. Their formation, dynamics and recombination can be followed by time-resolved mid-infrared spectroscopy. Measuring in the molecular fingerprint region to probe the samples allows the use of infrared activated vibrations as well as arising polaron bands [1].

Poly(3-hexylthiophene) (P3HT) is a popular and well-studied model system for organic photovoltaic materials. In a time-resolved mid-infrared spectroscopy study, we followed its polaron generation and recombination paths in comparison with the less common water-soluble derivative poly[3-(potassium-6-hexanoate)

thiophene] (P3P6T). Here, we found that different charge-carrier species such as polaron pairs and free polarons can be distinguished by the spectral position of their respective infrared activated absorption in the mid-infrared fingerprint region. Thereby, we were able to follow the formation of polaron pairs in the polymers and the subsequent separation to free polarons. Comparing both samples showed that the recombination in the more crystalline P3HT mainly occurs via interchain paths whereas intrachain recombination dominates in the more amorphous P3P6T.

While the structure of perovskite photovoltaic materials is different to polymer systems, the principle charge generation processes are similar. The crystal structure of perovskites leads to two different polaron sizes: Large polarons expand-

ing over a large number of primitive cells and small polarons which form on a single primitive cell. In 3D perovskites like methylammonium lead iodide (MAPbI₃), we found different polaron bands in the mid infrared with distinct dynamics. These could be associated to trapping as a mechanism for polaron localisation.

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Gallium nitride (GaN) nanowires (NWs) are promising candidates for photocatalytic applications due to their high surface-to-volume ratio and their waveguide character. We propose a fully integrated photocatalytic device consisting of a highly efficient UV LED as photon-source and functionalized GaN NWs grown on top of the LED. The device can be driven in a pulsed operation mode. This reduces light-induced deactivation processes of the catalyst, which are a problem in many standard photocatalytic systems [1]. We investigated the influence of the GaN NW growth on the electroluminescence time constants of the device. Furthermore, depending on the NW geometry, an efficient out-coupling of the light by the NWs can be obtained.

The structural stability of GaN NWs under operational conditions in aqueous elec-

trolytes is a key requirement. In pure deionized water, the m-plane side walls of the NWs are slowly decomposed under intense illumination, while the c-plane top facet proved to be stable [2]. We show that photo-generated holes are responsible for the decomposition of the GaN. The NWs can be stabilized by protective shells. P-type GaN NWs proved to be stable due to their upward surface band bending. Additionally, the stability of GaN nanofins is investigated as they enable a direct comparison of different crystallographic side walls facets. Depending on the orientation of the substrate with respect to the fin direction, the nanofins exhibit either m- or a-plane side facets [3]. We found that the a-plane side walls are more stable than the m-plane facets.

Consequently, the use of other nanostructures for photocatalysis might be also

promising as they expose other crystallographic facets and enable an even higher surface-to-volume ratio. By electrochemical measurements, we compared NWs, nanofins and nanogrids in terms of stability, effective surface area and charge transfer into an aqueous electrolyte.

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Combining nano-optical systems with optically active two-dimensional materials has recently emerged as a fascinating topic to achieve new optical functionalities at the nanoscale [1].

In this contribution, we present investigations of light-matter interactions between transition metal dichalcogenide (TMD) monolayers and lithographically defined gold bowtie nanoantennas. By performing 3D-FDTD calculations, we tuned the design of the bowtie nanoantennas to match the dipolar resonance with the fundamental exciton transitions in a proximal MoSe₂ monolayer. Fabricated bowtie nanoantennas show quality factors of $Q = 5$ and sub-10 nm feed-gaps with estimated mode volumes as small as $V_m = 2000 \text{ nm}^3$. Typical differential reflectance spectra recorded from individual TMD-bowtie nanostructures

at room temperature reveal low- and high-energy peaks separated by a dip at the energy of the uncoupled exciton.

To elucidate the nature of characteristic spectral features, we use the coupled oscillator model [2], which result in coupling constants at zero detuning of $g = 55 \text{ meV}$. This places our hybrid system in the weak-coupling regime with spectra exhibiting Fano-like behavior. Furthermore, we demonstrate active control of the optical response by varying the polarization of the excitation light. The methods developed in our work contribute to on-demand realization of optimally coupled TMD-nanoantenna systems that can be site-selectively addressed. This type of nanostructure could pave the way for on-chip actively controlled hybrid devices operating at elevated temperatures.

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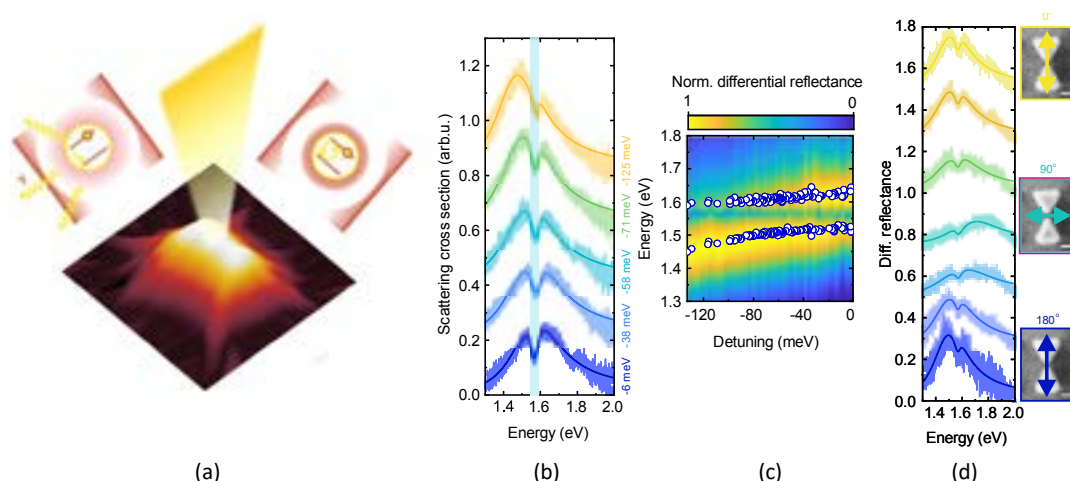


Figure 1: (a) Schematic representation of a TMD-bowtie hybrid nanostructure. (b)(c) Differential reflectance spectra recorded from single nanoantennas ordered by detuning to the exciton transition. Data reveals an anti-crossing-like behaviour. (d) Control of the optical response by tuning the polarization of the excitation light.

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Energy supply by fossil fuels only has a limited lifetime and is responsible for an increasing environmental pollution, influencing also climate change. A rapid transition to more sustainable solutions is thus also in the focus of modern research. Renewable fuels are meant to circumvent supply fluctuations arising from energy sources like PV and wind, at the cost of infrastructural adaptations. Direct renewable energy storage is thus highly desirable, but expansive and complicated.

Herein, we report an earth-abundant polymeric material, which for the first time enables the synergistic coupling of two key functions of energy conversion within one single material: visible light harvesting and electrochemical energy storage. The “solar battery” anode material, a 2D cyanamide-functionalized polyheptazine imide (NCN-PHI), is the first of its kind being capable of storing large amounts of photogenerated

electrons, operating even in aqueous conditions. Charge compensation and stabilization is realized by pseudocapacitive effects enabled by various aqueous alkali metal ions. Energetically, this occurs at energies well above the reversible hydrogen electrode, allowing for stable aqueous batteries with increased cell voltages [1].

The photogenerated, trapped charges can also be used to drive photocatalytic reactions like the Hydrogen evolution reaction in the absence of sunlight, a process called “dark photocatalysis”. Akin to natural photosynthesis, it allows decoupling the generation of fuels from the availability of light [2]. Exploiting both, the good photocatalytic and the charge storage properties, we show that NCN-PHI μ -particles can also be used as light propelled Janus particle microswimmers in different media, outperforming all other similar organic based systems.

In the right conditions, we show for the first time that it is possible to create a solar battery swimmer, which is propelled 25x longer than its illumination period. We anticipate that these findings are not only of high relevance for the storage of renewable energies, but also enable new applications in bio-compatible nanorobotics and drug delivery.

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SINGLET OXYGEN REACTIVITY WITH CARBONATE SOLVENTS USED FOR LI-ION BATTERY ELECTROLYTES

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In current lithium-ion batteries (LIBs), the formation of singlet oxygen was observed for layered transition metal (TM) oxide cathode active materials (CAMs, e.g. NCMs, HE-NCM) at high degrees of delithiation. This is accompanied by enhanced electrolyte decomposition, which is why this study focusses on the reactivity of chemically produced singlet oxygen with the commonly used cyclic and linear carbonate solvents for LIB electrolytes [1]. Additionally, electrolyte additives such as fluoroethylene carbonate (FEC) and difluoro ethylene carbonate (DiFEC) are investigated regarding their stability [2,3]. Using an on-line mass spectrometry setup, gassing during the decomposition of ethylene carbonate (EC), dimethyl carbonate (DMC), FEC and DiFEC is analyzed. Singlet

oxygen is produced in-situ by photoexcitation of a Rose Bengal dye. Ab initio calculations and on-the-fly simulations reveal a possible reaction mechanism for the reaction of EC with singlet oxygen via H_2O_2 and vinylene carbonate (VC) formation in the first reaction step. The formation of H_2O_2 is confirmed experimentally. In contrast to EC, simulations and experiments with DMC indicate stability in the presence of singlet oxygen. First experiments with FEC and DiFEC hint toward a possible thermal decomposition of FEC and stability of DiFEC toward singlet oxygen.

The produced H_2O_2 can already be electrochemically oxidized at potentials where singlet oxygen is formed, leading to protons and/or water, which both react with

the commonly used $LiPF_6$ conductive salt to HF. This, in turn, leads to TM dissolution from the CAMs, which is detrimental for the performance of a battery.

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PHOTO- AND ELECTROCATALYSIS BY TRANSITION METAL MABIQ COMPLEXES

36

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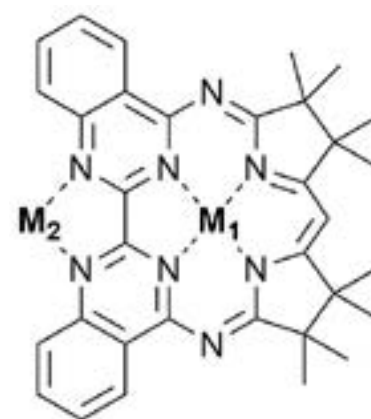
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In times of increasing energy demand, small molecule chemistry (e.g. CO_2 and O_2 activation; H_2 production) plays a central role in efforts to store renewable energy in chemical bonds. Molecular electrocatalysts and photosensitizers play an integral role in these processes. Photocatalysts have particular relevance for the production of solar fuels.

Research in our group centers on the development of such catalysts for small molecule chemistry. Toward this end, we have examined the coordination chemistry of a macrocyclic biquinazoline ligand (Mabiq). A series of first row transition metal-Mabiq complexes were synthesized and spectroscopically characterized, and their reactivity was examined. The $[Co^II(Mabiq)]^+$ com-

plex was subsequently examined as an electrocatalyst for hydrogen production. A range of electrochemical techniques was applied to study the mechanism of the hydrogen evolution reaction. The results illustrate the role of the “non-innocent” Mabiq ligand in this process.

Furthermore, the transition metal Mabiq complexes exhibit unique photochemical properties. The $[Zn^{II}(Mabiq)]^+$ complex is fluorescent, whereas the Ni-containing analogue can readily be photoreduced. The latter complex is an effective photoredox catalyst for the cyclization of a bromoalkyl-substituted indole. The application of the complexes in other photocatalytic reactions is currently being explored.



Mabiq complex

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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 $\text{Cs}_3\text{Bi}_2\text{I}_9$ 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.

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Organic-inorganic metal halide perovskite based solar cells (PSCs) are currently intensely researched for their potential as cheap and highly efficient next generation solar cells. Reaching module efficiencies of around 17% in 2018 [1], further improvement on upscaling is needed in order to push PSCs to commercialization. Especially changing the deposition method from lab-scale spin-coating to industrial compatible methods raises many questions due to the additional requirements, e.g. fast and roll-to-roll compatible deposition, low energy and low temperature processing as well as low material waste during production [2].

In principle, those requirements can be met by roll-to-roll slot-die coating [3–5]. Highly crystalline and uniform films with low defect concentrations are paramount in reaching high power conversion efficiencies in PSCs [6, 7].

A more detailed understanding of the perovskite crystallization process is needed for optimal film quality and hence high power conversion efficiencies using large area deposition techniques. 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 [8, 9].

In order to better understand crystallization kinetics of perovskite materials in-situ GISAXS and *in situ* GIWAXS measurements were done on methyl ammonium lead iodide (MAPI) thin films during printing. Thereby, the drying and crystallization kinetics were investigated for different printing temperatures. MAPI was printed on a glass/ITO/PEDOT:PSS layer structure in order to retrieve data relevant for real solar cell operation and facilitate comparison to existing working devices.

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CALCULATING OPTOELECTRONIC PROPERTIES OF HALIDE PEROVSKITES WITH A FIRST-PRINCIPLES TIGHT-BINDING APPROACH

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Solar cells based on halide perovskites (HaPs) have reached enormous power conversion efficiencies in a short amount of time and are already close to the performance of silicon devices. This is due to the fascinating properties of HaPs that are still not completely understood. In particular, it is a crucial open question how the outstanding optoelectronic properties can arise despite the remarkably soft lattice of HaPs. Theoretical calculations can provide important structure-function relations to address this question, but their applicability is often limited by their computational costs.

Our aim is to develop a theoretical formalism that enables calculating the properties HaPs at lower computational costs. This is needed in order to consider large super cells and nuclear dynamics required for the calculation of optoelectronic properties of HaPs at practically relevant con-

ditions. The use of conventional theoretical methods, such as density functional theory (DFT), can be challenging when investigating the interrelation of nuclear dynamics and optoelectronic features of HaPs. For this reason, we suggest a tight binding (TB) approach, which presents an efficient tool to model large-scale system sizes, since its computational complexity is heavily reduced compared to DFT. Specifically, we develop a TB parametrization based on DFT for the HaP methylammonium lead bromide, following previous work on methylammonium lead iodide [1].

This is done by projecting the Bloch wave functions on the basis functions corresponding to specific orbital sites of the atoms. The theoretical method provides us with the opportunity to study the impact of ionic composition and structural dynamics on optoelectronic characteristics of HaPs. Moreover, we can extend this approach to

rapid calculations of optoelectronic properties that include the dynamics of charge carriers at finite temperature.

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Secondary batteries are a key component for intermittent energy storage and e-mobility in the current energy transition. The state-of-the-art technology is based on Li-ion cells containing liquid electrolytes. All-solid-state batteries (ASSB) present a potential next-generation technology, promising increased operation safety and lifetime. The performance of solid-state electrolytes (SSE) in ASSBs, though, is severely limited by poorly understood interfacial processes either *in operando* during charge and discharge, or during high-temperature synthesis [1]. Atomistic insight into the structures, transport, and degradation processes at SSE grain boundaries (GB) [2] is thus crucial to rational advances in ASSB technology.

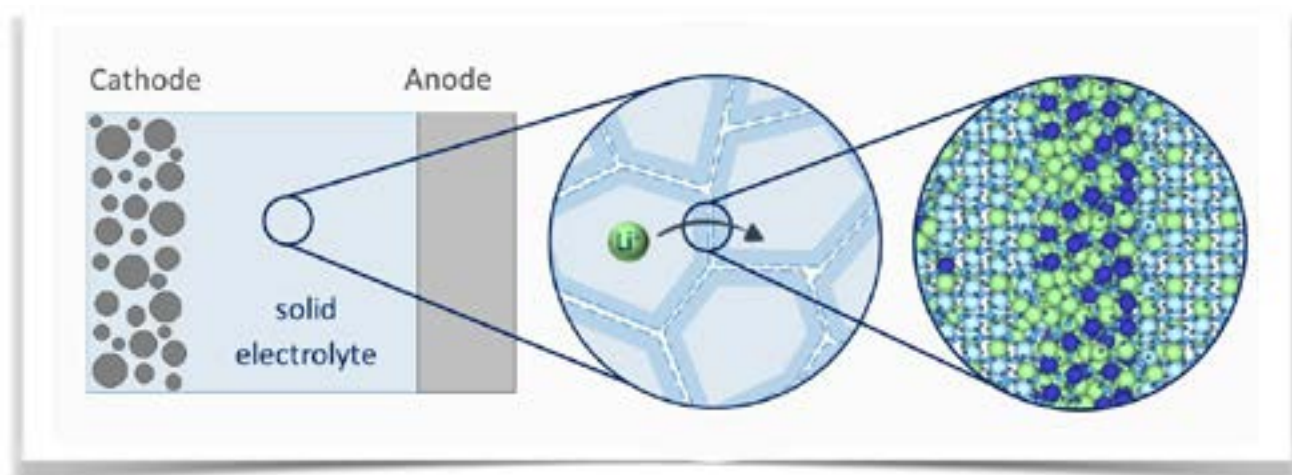
We apply molecular dynamics simulations (MD) with a first-principles derived force field to study GBs in the SSE LATP ($\text{Li}_{(1-x)}\text{Al}_x\text{Ti}_{(2-x)}(\text{PO}_4)_3$, $x=0.3$). An experimen-

tally guided simulation protocol is established to model GB formation during sintering. Anisotropic compression at high pressure and temperature leads to a loss of periodic structure at the interface. The obtained semi-amorphous domain is in agreement with findings from experimental TEM studies [3]. Structural scoring of simulated [4] and experimental TEM images confirms the co-existence of bulk-like and metastable interphases. Extensive sampling is reduced to glassy regions. The resulting GB structural models enable the investigation of lateral and transverse ion transport and the comparison to macroscopic properties.

With this approach, we leverage experimental input for modeling realistic solid-solid working interfaces [3] and explore the glassy configuration space by accelerated statistical sampling of structural ensembles through computational means.

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The reduction of CO₂ is a promising approach to establish a new C1 feedstock. An environmentally friendly procedure for this synthesis utilizes sunlight to provide the required energy [1]. The reduction of CO₂ to CO can be performed with Re(I)-catalysts which are able to act as photosensitizer, oxidation site, and reduction site [2]. Despite the benefits of excellent selectivity and high quantum yields these complexes show low stability under irradiation [3].

Understanding the mechanistic background and deactivation processes of the catalytic system is crucial to improve the system's turnover numbers (TONs), turnover frequencies (TOFs) and quantum yields (Φ). Herein, two deactivation processes both originating from the one-electron-reduced species (OER) of the catalyst

are presented. The light-induced excitation of the OER seems to cause deactivating side reactions. In the radical-induced pathway a quencher radical is assumed to combine with the OER [4]. We found two promising approaches to suppress these deactivation pathways. The use of pulsed light can decrease the irradiation of the OER-species, and therefore, increase the stability of the catalyst [5]. By adding the base 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) to the photocatalytic system and reducing the amount of the sacrificial electron donor Triethanolamine (TEOA), the likelihood of deactivation processes involving TEOA radicals can be decreased [6].

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IMPROVING THE BULK EMISSION PROPERTIES OF CH₃NH₃PbBr₃ BY MODIFYING THE HALIDE-RELATED DEFECT STRUCTURE

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The outstanding potential of halide perovskite for optoelectronic devices has been widely demonstrated over the past years. In particular, the defect chemistry of hybrid organic–inorganic lead halide perovskites is believed to be partially responsible for the optical performance of this solution-processed material. In this work, the role of bromine-based defects on the emission properties of CH₃NH₃PbBr₃ is investigated.

Herein, micron sized single crystals are analyzed to study effects on surface and bulk emission as they are exposed to bromine vapors. We follow the evolution of the emission by means of photoluminescence

(PL) microscopy as well as spectral and time resolved measurements. This allows us to carry out a complete analysis with spatial, spectral and temporal resolution of the emission from these systems. Through this study we find evidence for a strong PL improvement through bromine vapor treatment which remains for tens of hours. We observe bromine penetration into the material which positively affects bulk emission. A defect-related mechanism behind this improvement is proposed which takes into account crystal orientation and the nature of bromine defects as deep or shallow traps. Furthermore, an insight on spatial distribution of light emission origins in the material is given.

With these results we help understand the defect structure in these materials and present a post-fabrication method to improve the emission throughout the entire volume of CH₃NH₃PbBr₃ in the absence of appreciable degradation.

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Understanding the charge transport properties of organic-inorganic interfaces is crucial for the development and improvement of molecular electronic devices. Often gas phase properties of molecules are used to predict the conductance properties of molecular assemblies. However, dipole moments along the molecular backbone lead to collective electrostatic effects in densely packed self-assembled monolayers (SAMs). Such effects are affecting the level alignment and transport properties of SAM-based devices and, consequently, rendering the gas phase predictions inaccurate or even invalid.

In our recent work [1], we combined experiments and first-principles calculations

based on density functional theory to study the impact of collective electrostatic effects on the transport properties of aromatic thiol-biphenyl-based SAMs with hydrogen and various halogen terminations on Au. Through the dipole moments introduced by the halogen termination at the tails of the molecular backbones, we observe large modifications of the work-functions.

Furthermore, we find that the modification of the work-function is significantly lower for the halogen terminated SAMs as compared to the hydrogen terminated interface. Experimentally, we show that these differences between hydrogen and halogen terminated SAMs result in the current

being one order of magnitude larger for the former. Furthermore, our computations reveal that this transport characteristic of the different SAMs arises from a complex interplay between dipole moments along the interface and backbone, leading to a lowering of the tunneling barrier for the hydrogen compared to the halogen terminated SAMs.

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TUNING OXYGEN EVOLUTION ACTIVITY AS A FUNCTION OF COMPOSITION: A CASE STUDY OF NEW IRIDATE-RUTHENATE LAYERED OXIDES FROM $\text{Na}_2\text{Ir}_{1-x}\text{Ru}_x\text{O}_3$

S. Laha, M. A. Plass, V. Duppel, S. Bette, R. Dinnebier, Nella M. Vargas-Barbosa, B. V. Lotsch

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We recently reported highly active exfoliated iridate and ruthenate nanosheets as stable electrocatalysts for the oxygen evolution reaction (OER) in acidic medium derived from the layered $\text{K}_{0.75}\text{Na}_{0.25}\text{IrO}_2$ and NaRuO_2 compounds [1,2]. The nanosheets are among the best performing catalysts both in terms of specific and mass activity, which may allow cost-effective electrode design at low noble metal catalyst loading for PEM. It was recently proposed that surface segregation can aid the design of stable noble metal oxides for the OER.[3]

Here, we explore such an effect by characterizing the electrocatalytic activity and stability of mixed Ir-Ru layered oxides, $\text{H}_3\text{NaIr}_{2-2x}\text{Ru}_{2x}\text{O}_6$ ($0 \leq x \leq 1$). Starting from the

parent compound Na_2RuO_3 , we prepare solid-solutions of $\text{Na}_2\text{Ir}_{1-x}\text{Ru}_x\text{O}_3$, acid exchange them and then disperse them prior to drop-casting onto glassy carbon electrodes for characterization. In general, we observe a composition-dependent trend for the performance (overpotential at specific current densities) of the catalysts. Similarly, the stability of the catalysts is greatly affected by the composition. Our electrochemical characterization is complemented by electron microscopy, X-ray diffraction as well as ex-situ spectroscopic methods to truly assess the structure-property relationships of this class of materials.

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$\text{Cu}_9\text{Te}_4\text{Cl}_3$ AND $\text{Ag}_{10}\text{Te}_4\text{Br}_3$ - INVESTIGATION OF P - N - P -SWITCHING IN THERMOELECTRIC COMPOUNDS

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Polymorphism is a common observed phenomenon in solid materials, often accompanied by a change of properties undergoing the phase transitions. The class of materials designated the 'p-n-p-compounds' is a class of ion conductors capable of reversible switching between p- and n-type of semi conduction.

These compounds undergo mobility-driven order-disorder phase transitions, showing typical phonon softening effects and modulations in the thermoelectric properties. This has been confirmed to be usually attended by closing of the band gap and increasing in the density at the fermi level leading to an intermediate quasi-metallic state, in which valence electron conduction increases [1,2]. The structure features leading to pnp-switching are carved out by the comparison of the 'p-n-p-compound' $\text{Ag}_{10}\text{Te}_4\text{Br}_3$ with the structurally closely related copper polytelluride chlo-

rides $\text{Cu}_{9,1}\text{Te}_4\text{Cl}_3$ and $\text{Cu}_{9,5}\text{Te}_4\text{Cl}_3$. $\text{Ag}_{10}\text{Te}_4\text{Br}_3$ undergoes p-n-p-switching accompanied by a huge jump of the Seebeck coefficient released by the variation of temperature [3-6].

The structurally closely related compounds $\text{Cu}_{9,1}\text{Te}_4\text{Cl}_3$ and $\text{Cu}_{9,5}\text{Te}_4\text{Cl}_3$ also show polymorphism, but do not exhibit any p-n-p-switching or discontinuities of the Seebeck coefficient. The thermoelectric figure of merit ZT is one order of magnitude higher in the copper compounds.

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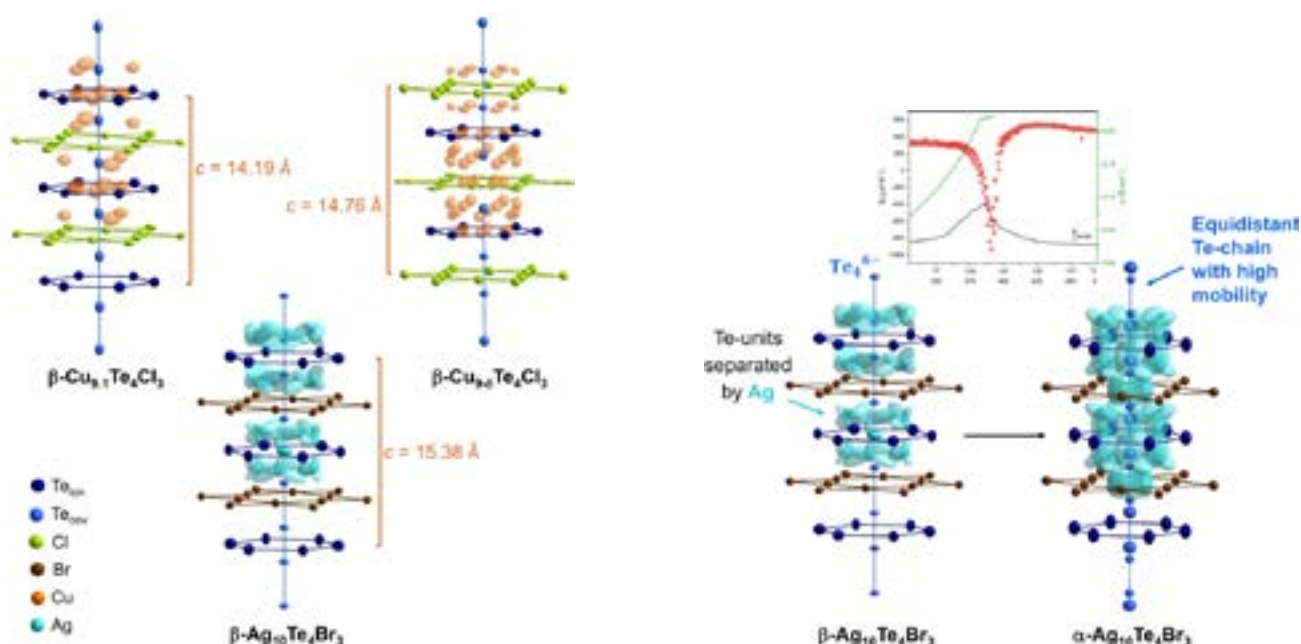
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Understanding the energetic and electric nature of interfaces plays a major role in the development of semiconductor devices. One of the most common representatives are *p-n* junctions, which cause charge carrier separation by the formation of a space charge region and therefore are the centerpiece in solar cells.

In order to improve the understanding of these interfaces, we investigate a simplified model within one material: We succeed to produce one to two monolayers thin, crystalline organic films of a perylene diimide with grain sizes up to several hundred microns. The grain boundary in between acts as interface where the formation of an energetic barrier or valley is predicted theoretically [1]. We investigate the energetics of those grain boundaries by Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) [2].

We find that indeed grain boundaries act as thin layer with a different Fermi energy compared to the neighboring grains, thereby creating a space charge region. This relative energy difference we find to take positive or negative values, therefore acting as energy barrier or valley for the charge carriers, respectively. We observe that the change in molecular orientation at this grain boundary correlates with the absolute value of this energy difference. Furthermore, we see a clear dependence on charge carrier density within the organic film, which we change by illumination with visible light and back gate voltage.

With these results, we can aim for the manipulation of electric current by photocurrent measurements using light of the far infrared (FIR-PC).

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METAL-ORGANIC FRAMEWORKS (MOFs) AS PROSPECTIVE HYBRID MATERIALS IN OPTICAL APPLICATIONS

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NLO effects such as multi-photon absorption, have a wide range of applications (optical limiting, fluorescence excitation microscopy, three-dimensional data storage) [1]. These effects have been studied in several material classes including a variety of different organic dye molecules as well as inorganic particles [2-3]. However, often these material are limited towards their applicability due to unfavourable inherent properties such as toxicity and restricted tunability of wavelength [1].

Inorganic-organic solid-state hybrid materials (coordination polymers (CP), metal-organic frameworks) have the great potential to overcome those problems. One prominent example are their luminescence properties, since the incorporation of chromophore linker molecules into

the solid material increases the emission properties by reduction of non-radiative energy decay. Additionally to this significant advantage of MOFs and CPs compared to molecular materials, an uncontrolled aggregation of chromophores in a highly concentrated solutions – leading to fluorescence quenching [4] – is prevented while a high chromophore density is enabled. Our group is focussing on MOFs and their photophysical properties as well as processes of energy transfer inside the materials. Our approach is to synthesize organic dye molecules as chromophores, incorporate them in solid-state hybrid materials (MOFs and CPs) and investigate their properties to deepen the understanding towards a structure-(photophysical-) property relationship.

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In the design and fabrication of micro-patterned optically active devices, characterization methods that go beyond the bulk optical response are highly attractive. In these settings, an ideal experiment directly correlates the response and function with local structure. We here target such correlation of local structure and function by implementing a fast and versatile Fourier-transform photocurrent micro-spectrometer operating in the visible and near-infrared spectral range.

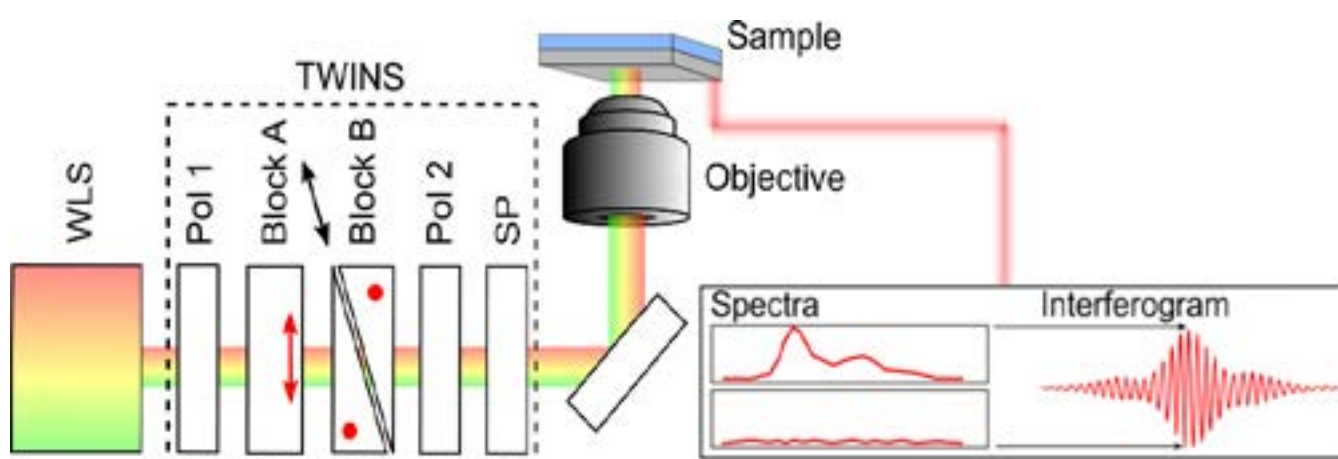
We obtain photocurrent interferograms by focusing a white-light supercontinuum modulated by a common-path interferometer (TWINS [1-4]) onto a device with a microscope objective. The common-path design of the interferometer, relying on birefringent wedges to generate two phase-locked beam replicas with tunable phase-delay, retains all advantages of broadband

Fourier-transform spectroscopy while circumventing the need for e.g. active stabilization [3]. The final implementation allows diffraction-limited mapping of photocurrent excitation spectra, directly showing how the optical response changes across the sample.

We performed a proof of principle experiment on a dual-gated GaAs dummy device. The sample was contacted with dual-gated titanium-gold contacts positioned in a finger structure with 6 μm separation, allowing read-out of photocurrent under illumination. During the experiment, we illuminate the biased sample with 500-950 nm light while measuring photocurrent as a function of interferometer phase-delay at several separate spatial areas. By Fourier-transforming the resulting interferograms we obtain local photocurrent excitation-wavelength dependence in the device.

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Schematic representation of the photocurrent micro-spectrometer. The supercontinuum output of a FIANIUM laser is modulated by a common path interferometer (TWINS), and focused into a diffraction limited spot on the sample. We read out a photocurrent interferogram from the sample device, which can be Fourier transformed to yield a photocurrent excitation spectrum.

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One of the key factors limiting the widespread applications of fuel cell technologies is the cost of the electrocatalysts utilized in catalyzing the oxygen reduction reaction (ORR) at the cathode side. Only platinum based electrocatalysts have shown sufficient activity; however, due to the scarcity and cost of Pt, it is of a particular interest to increase their activity per mass. We tackle these challenges by combining theory and experiment to fabricate pure Pt nanoparticles with optimal size and shape. Optimal nanoparticle sizes are predicted ~1, 2, and 3 nm by computational screening. We synthesized the 1 nm sized Pt nanoparticles with metal organic framework template approach. The observed mass activities ($0.87 \text{ A/mg}_{\text{Pt}}$) coincide with the computational predic-

tion ($0.99 \text{ A/mg}_{\text{Pt}}$) and represent one of the highest mass activities reported among pure Pt catalysts for the ORR.

Theoretical calculations have also demonstrated that optimal shapes for the Pt nanoparticles are the ones with a highly defective surface, e.g., containing concave surface sites. We developed one-step top-down approach to produce Pt/C catalyst (with 3 nm Pt NP diameter).

Results of high-resolution transmission electron microscopy and tomography, electrochemical techniques revealed the evidence of a high density of surface defects. The ORR activity of the developed catalyst was $0.71 \text{ A/mg}_{\text{Pt}}$. Moreover, the new technique reduces the complexity of

the synthesis compared to state-of-the-art bottom-up techniques.

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- [3] J. Fichtner, S. Watzele, B. Garlyyev, A. S. Bandarenka, in preparation

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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 MAPbI₃ and MAPbBr₃ 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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Energy conversion devices based on the organic-inorganic tri-halide perovskite family of materials have shown great potential due to their low cost as well as reasonably high power conversion efficiencies [1]. However, a major concern is the stability of these materials, which hinders device performance under realistic environments [2]. A similar material platform are two-dimensional (2D) Ruddlesden-Popper halide perovskites stoichiometric ratios are defined by the general formula $A_2A'_{n-1}M_nX_{3n+1}$ where A, A' are cations, M is a metal, X is a halide and the integer value n determines the perovskite layer thickness (or quantum well thickness). These materials can be solution processed, reveal similar solar cell efficiencies and stability approaching technological relevance. Further, the optoelectronic properties can be tuned widely

across the visible range by changing the perovskite layer thickness [4].

However, fundamental questions concerning optical resonances and ultimate material quality and stability are still topic of current research. Here, we improve the material stability and optical properties of excitons in $(BA)_2(MA)_{n-1}Pb_nI_{3n+1}$ by encapsulation of exfoliated crystals in atomically flat hexagonal boron nitride (hBN). We improve the linewidth of photoluminescence to the point where we reveal spectral features which are consistent with monolayer thickness fluctuations of the perovskite quantum well. Spatial correlation analysis reveal the length scale of these monolayer fluctuations and will guide improvements in material synthesis.

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List of Participants

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Mahshid	Alizadeh	Ludwig-Maximilians-Universität München	01	I (Tuesday)
Tayebeh	Ameri	Ludwig-Maximilians-Universität München		
Tina	Angerer	Technische Universität München		
Aliaksandr	Bandarenka	Technische Universität München		
Thomas	Bein	Ludwig-Maximilians-Universität München		
Alexander	Biewald	Ludwig-Maximilians-Universität München	02	I (Tuesday)
Ardemis	Boghossian	EPFL, Lausanne		
Alexander	Bourgund	Technische Universität München	03	I (Tuesday)
Ali	Buyruk	Ludwig-Maximilians-Universität München	04	I (Tuesday)
Ib	Chorkendorff	Technical University of Denmark		
Emiliano	Cortés	Ludwig-Maximilians-Universität München		
Marcel	Dann	Ludwig-Maximilians-Universität München	05	I (Tuesday)
Regina	de Vivie-Riedle	Ludwig-Maximilians-Universität München		
Fabio	del Giudice	Technische Universität München	06	I (Tuesday)
Felix	Deschler	Technische Universität München		
Xing	Ding	Technische Universität München	07	I (Tuesday)
Hubert	Ebert	Ludwig-Maximilians-Universität München		
David	Egger	Technische Universität München		
Rüdiger-A.	Eichel	Forschungszentrum Jülich		
Johanna	Eichhorn	Technische Universität München	08	I (Tuesday)
Clara	Eisebraun	Technische Universität München	09	I (Tuesday)
Florian	Engelsberger	Ludwig-Maximilians-Universität München	10	I (Tuesday)
Jochen	Feldmann	Ludwig-Maximilians-Universität München		
Jonathan	Finley	Technische Universität München	33	II (Thursday)
Philipp	Fischer	Technische Universität München	11	I (Tuesday)
Roland	Fischer	Technische Universität München		
Sergej	Fust	Technische Universität München	12	I (Tuesday)
Batyr	Garlyyev	Technische Universität München	49	II (Thursday)
Christian	Gehrmann	Technische Universität München	13	I (Tuesday)
Nadja	Giesbrecht	Ludwig-Maximilians-Universität München	14	I (Tuesday)
Justin	Gooding	UNSW Sydney		
Moritz	Gramlich	Ludwig-Maximilians-Universität München	50	II (Thursday)
Theresa	Grünleitner	Technische Universität München	15	I (Tuesday)
Marcella	Günther	Ludwig-Maximilians-Universität München	16	I (Tuesday)
Ren-jun	Guo	Technische Universität München	17	I (Tuesday)
Anders	Hagfeldt	EPFL, Lausanne		
Dan	Han	Ludwig-Maximilians-Universität München	18	I (Tuesday)
Achim	Hartschuh	Ludwig-Maximilians-Universität München		
Juergen	Hauer	Technische Universität München		
Ulrich	Heiz	Technische Universität München		
Laura	Herz	University of Oxford		
Corinna	Hess	Technische Universität München		
Theresa	Hoffmann	Technische Universität München	32	II (Thursday)
Alexander	Holleitner	Technische Universität München		
Nicolas	Hörmann	Technische Universität München	19	I (Tuesday)
Alexander	Hötger	Technische Universität München	20	I (Tuesday)
Ivan	Huc	Ludwig-Maximilians-Universität München		
Ludwig	Hüttenhofer	Ludwig-Maximilians-Universität München	21	I (Tuesday)
Hristo	Iglev	Technische Universität München		
Joanna	Kargul	University of Warsaw		
Julian	Klein	Technische Universität München	22	I (Tuesday)
Axel	Knop-Gericke	MPI for Chemical Energy Conversion		
Gregor	Kobl Müller	Technische Universität München	24	I (Tuesday)
Bernhard	Kretz	Technische Universität München	43	II (Thursday)
Katharina	Krischer	Technische Universität München		
Viktoria	Kunzelmann	Technische Universität München	25	I (Tuesday)

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Barbara	Lechner	Technische Universität München		
Tim	Liedl	Ludwig-Maximilians-Universität München		
Ru-Shi	Liu	NTU Taipeh		
Maria Antonietta	Loi	University of Groningen		
Yueh-Lin	Loo	University of Princeton		
Bettina	Lotsch	MPI for Solid State Research		
Thomas	Lunkenbein	Fritz-Haber-Institut der MPG		
André	Mähringer	Ludwig-Maximilians-Universität München	26	II (Thursday)
Joachim	Maier	MPI for Solid State Research		
Stefan	Maier	Ludwig-Maximilians-Universität München		
Thomas	Maier	Technische Universität München	28	II (Thursday)
Dimitrios	Manganas	MPI für Kohlenforschung	27	II (Thursday)
David	Mayer	Technische Universität München	29	II (Thursday)
Philipp	Moser	Technische Universität München	51	II (Thursday)
Peter	Müller-Buschbaum	Technische Universität München		
Ron	Naaman	Weizmann Institute of Science, Israel		
Linda	Nazar	University of Waterloo		
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Tom	Nilges	Technische Universität München		
Jens	Nørskov	Technical University of Denmark		
Matthias	Nuber	Technische Universität München	31	II (Thursday)
Harald	Oberhofer	Technische Universität München		
Christian	Ochsenfeld	Ludwig-Maximilians-Universität München		
Florian	Pantle	Technische Universität München	32	II (Thursday)
Annamaria	Petrozza	IIT Genova		
Filip	Podjaski	MPI for Solid State Research	34	II (Thursday)
Svitlana	Polesya	Ludwig-Maximilians-Universität München	18	I (Tuesday)
Simon	Qian	Technische Universität München	35	II (Thursday)
Karsten	Reuter	Technische Universität München		
Kerstin	Rickmeyer	Technische Universität München	36	II (Thursday)
Bernhard	Rieger	Technische Universität München		
Sebastian	Rieger	Ludwig-Maximilians-Universität München	37	II (Thursday)
Gökçen	Savasci	Ludwig-Maximilians-Universität München		
Manuel	Scheel	Technische Universität München	38	II (Thursday)
Christoph	Scheurer	Technische Universität München		
Maximilian	Schilcher	Technische Universität München	39	II (Thursday)
Wolfgang	Schnick	Ludwig-Maximilians-Universität München		
Ram	Seshadri	University of California, Santa Barbara		
Ian	Sharp	Technische Universität München		
Sina	Stegmaier	Technische Universität München	40	II (Thursday)
Andreas	Stier	Technische Universität München	23	I (Tuesday)
Jacek	Stolarczyk	Ludwig-Maximilians-Universität München		
Christopher	Thomas	Technische Universität München	41	II (Thursday)
Erling	Thyrhaug	Technische Universität München	48	II (Thursday)
David	Tiede	Universität Münster	42	II (Thursday)
Philip	Tinnefeld	Ludwig-Maximilians-Universität München		
Sefaattin	Tongay	Arizona State University		
Alexander	Urban	Ludwig-Maximilians-Universität München		
Chris	Van de Walle	University of California, Santa Barbara		
Nella	Vargas-Barbosa	MPI for Solid State Research	44	II (Thursday)
Anna	Vogel	Technische Universität München	45	II (Thursday)
Lisa	Walter	Ludwig-Maximilians-Universität München	46	II (Thursday)
Sebastian	Weishäupl	Technische Universität München	47	II (Thursday)
Thomas	Weitz	Ludwig-Maximilians-Universität München		
Lukas	Wolz	Technische Universität München	48	II (Thursday)

	Monday, Sep 9	Aula Magna		Tuesday, Sep 10	Aula Magna		Wednesday, Sep 11	Aula Magna		Thursday, Sep 12	Auditorium		Friday, Sep 13	Aula Magna
09:35	Welcome Address		09:35	Yueh-Lin Loo Understanding and Influencing Structural Evolution in Morphologically Complex Semiconductors for Photovoltaic Applications	p. 15	09:35	Ardemis Boghossian A NanoBioengineering Approach to Developing Living Photovoltaics	p. 20	09:35	Jens K. Nørskov Electrochemical Ammonia Synthesis	p. 24	09:35	Felix Deschler Ultrafast Spectroscopy of Charge and Structural Dynamics in Hybrid Perovskites	p. 30
09:45	Anders Hagfeldt Composition and Interface Engineering of Perovskite Solar Cells	p. 8	10:20	J. Justin Gooding Nanozymes: Nanoparticles that Mimic Enzyme Architecture for the Oxygen Reduction Reaction and the Carbon Dioxide Reduction Reaction	p. 16	10:20	Maria Antonietta Loi Sn-based Hybrid Perovskites: from Solar Cells to Hot Electrons	p. 21	10:20	Poster Session II & Coffee (Grecalle Building)		10:05	Chris G. Van de Walle First-Principles Studies of Radiative and Nonradiative Recombination in Halide Perovskites	p. 31
10:30	Gregor Kobl Müller Semiconductor Nanowires for Thermoelectric Energy Conversion	p. 9	11:05	Coffee Break (Lobby)		11:05	Coffee Break (Lobby)		10:50	Closing Remarks				
11:00	Coffee Break (Lobby)		11:35	Ib Chorkendorff Electrochemical Conversion of Sustainable Energy	p. 17	11:35	Laura M. Herz Dynamics of Charge-Carriers and Ions in Metal Halide Perovskites for Solar Cells	p. 22	11:15	End of Conference				
11:30	Joachim Maier Ionic and Electronic Charge Carriers in Solids: Implications for Energy Conversion and Storage	p. 10	12:20	Ron Naaman The Electron Spin and Chiral Molecules - Together They Make the Difference	p. 18	12:20	Tayebah Ameri Morphology Analysis and Interface Engineering of Solution-Processable Photovoltaics	p. 23						
12:15	Ram Seshadri Using computation to Guide Energy Materials Discovery	p. 11	13:05	Lunch Break		13:05	Lunch Break & Informal Discussions		12:50	Lunch Break				
13:00	Lunch Break		14:15	David A. Egger Connections between Structural Dynamics and Optoelectronic Properties of Halide Perovskites from First-Principles Calculations	p. 19				14:15	Ru-Shi Liu Narrow Emission Band Phosphors for Application in High-Power LEDs	p. 25			
14:30	Annamaria Petrozza Understanding Defect Physics to Stabilize Metal-Halide Perovskite Semiconductors for Optoelectronic Applications	p. 12	14:45	Poster Session I & Coffee, Drinks and Snacks (Lobby, 14:45 - 17:15)					15:00	Joanna Kargul Rational Approaches to Engineering Direct Electron Transfer in Photosystem I-based Biophotoelectrodes	p. 26			
15:15	Linda F. Nazar Understanding and Enhancing Ion Transport in Solids and at Interfaces for All-Solid-State Lithium and Sodium Energy Storage	p. 13							15:45	Coffee Break (Grecalle Building)				
16:00	Coffee Break (Lobby)								16:15	Sefaatin Tongay The Synthesis of Exotonic Grade 2D Janus Crystals	p. 27			
16:30	Harald Oberhofer How Does Molecular Structure Influence Charge Mobility? Mining a Database of Organic Semiconductors	p. 14							17:00	Stefan A. Maier Plasmonic Nanoparticles as Energy Converters for Chemical Reactions and for the Launching of Acoustic Surface Waves	p. 28			
17:00	Welcome Reception (Lobby)								17:30	Rüdiger-A. Eichel Advanced Batteries – Electrochemistry at Interfaces and Interphases	p. 29			
									18:30	Conference Dinner (Grecalle Building)				

SCHEDULE