Turning points in the energy transition: Setting the course for the next decades

12th Energy Colloquium of the Munich Institute of Integrated Materials, Energy and Process Engineering (MEP)

July 28, 2022

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With the Russian invasion of Ukraine, a whole new chapter of European and especially German energy policy has begun.

Germany's ever-increasing dependence on Russian energy imports will now decline abruptly or steadily, and entirely new energy policy paths will have to be found. Whether there will now be an accelerated transformation of the energy system towards renewable energy or a reversion to the use of coal and oil is now unclear.

The fact that the lessons of the oil crises have been so neglected is frightening. In the 1970s, the International Energy Agency, an agency that was supposed to prevent such a political shortage crisis forever in the future, was established; unfortunately, this and many other institutions failed. The discussion of climate change dominated the situation - albeit understandably - and issues of geopolitics seemed topics of the past. Now, all of a sudden, the world is confronted with geopolitical dislocations again and, unfortunately, has not made much progress on the issue of climate change.

For energy research, this changes the pace at which solutions must be found. In order to reduce one-sided dependencies and to combat climate change quickly, there can only be a significant intensification of energy research. Energy research will thus become the central challenge in the coming years and decades. Research, industry and politics must enter into a new alliance so that practicable solutions are quickly available that are politically feasible, socially acceptable and ecologically well thought out over the entire life cycle.

Thomas Hamacher
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Munich Institute of Integrated Materials,
Energy and Process Engineering (MEP)

12th Energy Colloquium of the Munich Institute of Integrated Materials, Energy and Process Engineering (MEP)

Turning points in the energy transition: Setting the course for the next decades

28th July 2022
TUM Entrepreneurship Research Institute, Garching-Forschungszentrum

Register until 20th July 2022

Program

08:30 – 09:00 Registration & Poster hang-up

09:00 – 09:15 Opening
Prof. Dr. Thomas Hamacher
Munich Institute of Integrated Materials, Energy and Process Engineering, TUM

09:15 – 09:45 Keynote
Destination: Climate Neutrality – Navigating Theory and Practice
Moritz Limbacher
Dena (Deutsche Energie-Agentur)

09:45 – 10:45 Cross-Scale - Energy Management and Grids
Chair: Prof. Dr.-Ing. Andreas Jossen, Institute for Electrical Energy Storage Technology, TUM

Techno-Economic Analysis of Intercontinental Electricity Grids with Future European Energy System
Thushara Addanki, Chair of Renewable and Sustainable Energy Systems, TUM

A Simplified Microgrid Architechture with Reduced Number of Measurement Units
Prashant Pant, Chair of Renewable and Sustainable Energy Systems, TUM

Energy Management in Neighborhoods – A digital Platform Solution
Thomas Lickléderer, Munich Institute of Integrated Materials, Energy and Process Engineering, TUM

10:45 – 10:55 Coffee Break

10:55 – 12:25 Poster Session 1

12:25 – 13:30 Lunch Break

13:30 – 14:00 Keynote
The Potential of Waste Heat Recovery from Industry in Europe – an ORC Perspective
Dr.-Ing. Christoph Wieland
Chair of Energy Systems, TUM

14:00 – 15:00 Innovative Materials and Methods for Energy Solutions
Chair: Prof. Dr. Peter Müller-Buschbaum, Chair of Functional Materials, TUM

In Situ Investigation of Thermoelectric Thin Films Based on Ionic Liquid Post-Treated PEDOT:PSS
Anna Lena Oechsle, Chair of Functional Materials, TUM

Non-Uniform Lithium Distribution in 18650-Type Lithium-Ion Battery During Dis-/Charging
Dominik Petz, Chair of Functional Materials, TUM

Manufacturing of New Uranium Fuel for FRM II Conversion
Kevin Buducan, Research Neutron Source FRM II, TUM

15:00 – 16:30 Poster Session 2

16:30 – 16:40 Coffee Break

16:40 – 17:10 Keynote
Hydrogen as an important factor to support the energy transition
Dr. Stefan Spindler
CEO Industrial Schaeffler AG

17:10 – 17:50 Analytical Insights on Future Fuels
Chair: Prof. Dr.-Ing. Hartmut Spliethoff, Chair of Energy Systems, TUM

Insights into Current and Future Experimental Investigation of Conventional and Plasma-Assisted Solid Fuel Entrained Flow Gasification
Tobias Netter, Chair of Energy Systems, TUM

In-Situ Identification of Electrocatalytically Active Areas on Palladium Using Electrochemical Scanning Tunneling Microscopy
Thorsten O. Schmidt, Professorship of Physics of Energy Conversion & Storage, TUM

17:50 – 18:10 Award & Closing Ceremony

18:10 – 19:00 Socializing

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1. Oral Presentations

Energy management in neighborhoods - A digital platform solution

Lickleder Thomas[a], Mayer Jan[b], Bytschkow Denis, Capone Alexandre,
Kramer Michael, Thomas Hamacher[c]

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The energy supply of buildings plays an important role in the decarbonization of the energy system. Until now, the focus of energy management has been on individual buildings and the various sectors, such as electricity or heat, have usually been considered separately. With the aim of exploiting synergy effects and optimizing the efficiency of energy supply in neighborhoods, in the research project "Multi-Energy Management and Aggregation Platform (MEMAP)" a software environment was developed for cross-building and inter-sectoral energy management in neighborhoods during live operation.

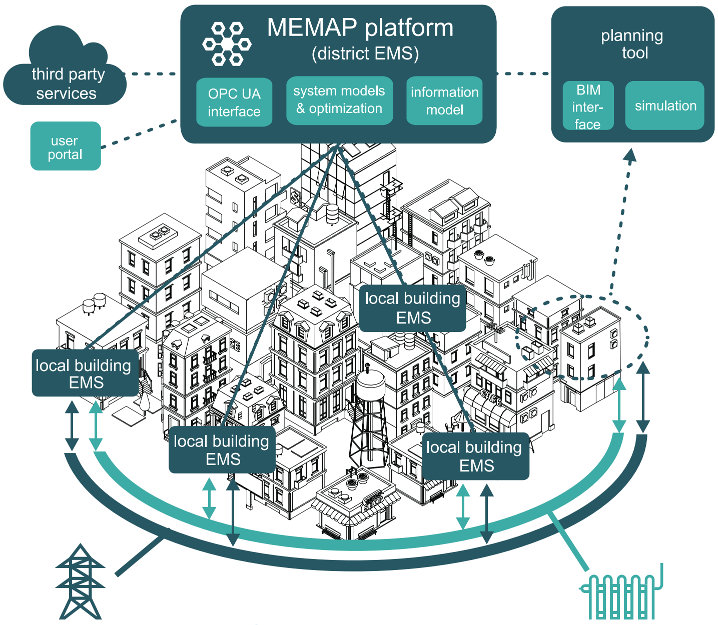

Figure 1: MEMAP Platform interconnection buildings in a district.

As an academic partner in the project consortium, the focus in the subproject of the Munich School of Engineering (MSE) of the Technical University of Munich (TUM) was on the modeling, optimization and simulation of the neighborhoods as multi-energy systems. A platform concept was developed for interconnecting local energy management systems (EMS) in the districts, using the OPC UA communication standard to aggregate data from the individual buildings. Based on this, abstract and transferable models were developed for representing the most relevant device classes in districts. In line with the current state of the art, these were embedded in the formulation of a model predictive controller (MPC) for the coupled optimization of electrical and thermal energy flows in the neighborhood. The MPC framework also allows to proactively consider forecasts of time-varying boundary conditions, such as volatile renewable energy generation, fluctuating prices, and load curves of consumers in the neighborhood. For example, price variations can be exploited automatically, and storage facilities can be charged or discharged proactively to minimize operating costs or CO2 emissions. The formulation and solution of the associated mixed integer linear (MILP) optimization problem was automated with the project partners in a Java-based software implementation. This was complemented by a developed information model and communication concept for live operation, resulting in the MEMAP platform as a prototype of a digital district energy management solution. The laboratory for Combined Smart Energy Systems (CoSES) at TUM was used as a test environment. Here, the practicality of the interfaces was realistically demonstrated, and the functionality of the developed concepts and software artifacts was validated in experiments with real hardware devices that can typically be found in neighborhoods.

The source code of the developed MEMAP platform and planning tool is available in a GitLab repository under open-source license (https://git.fortiss.org/ASCI-public/memap). The project results, as well as findings, are described in detail in the final project report [1]. With the MEMAP platform as a tool for optimized energy management in neighborhoods and the accompanying studies, the project has thus contributed to the energy efficiency of neighborhoods and their sustainable energy supply.

References

[1] Licklederer et al., Abschlussbericht „Multi-Energie Management und Aggregationsplattform (MEMAP)“ der TU München, 2022, https://mediatum.ub.tum.de/1658818

A Simplified Microgrid Architecture with Reduced Number of Measurement Units

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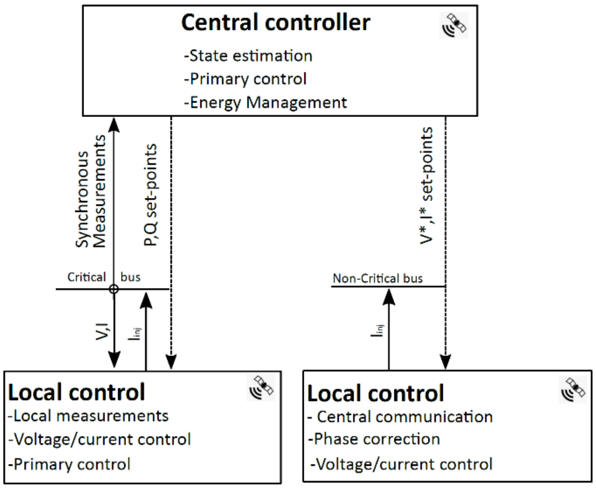
Smart microgrid concept assumes large penetration of power electronics interfaced distributed energy resources. The efficient and reliable control of such micro-grid requires full system observability. However, deploying multiple measurement units in small low-voltage micro-grids increases the overall cost of system This work, proposes a simplified central-controller based micro-grid architecture as shown in Fig.1, that eliminates the need for local measurements traditionally used for inverter synchronization and control, instead relies upon state-estimation (at central-controller) and GPS time-synchronization (at the local controller)



Central controller
-State estimation
-Primary control
-Energy Management

Local control
-Local measurements
-Voltage/current control
-Primary control

Local control
- Central communication
-Phase correction
-Voltage/current control

Figure 1: Proposed microgrid architecture

The proposed architecture (without inverter local measurements) is compared against a reference case (with all the measurements) in Typhoon HIL simulator as shown in Fig.3. Load 2 is increased to 5 kW, bus 3 voltage and inverter response is shown in Fig.3 and 4 respectively.

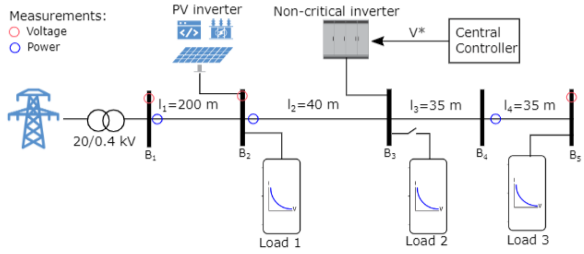


Figure 2: Simulation configuration

Key observations:

- Due to communication delay voltage estimation is slightly delayed, hence the inverter active power response (P-V droop) is also delayed.
- The proposed architecture is a trade-off between measurement costs and reduced response rate of inverters.

Local controllers receive voltage/current reference from the central-controller. To ensure time synchronization, the local controller compensates for the time delay caused by communication and central controller operation.

If V_x is the estimated voltage at central controller,

$$V_x = V_m \cdot \cos(\omega t + \varphi_{vx}),$$

corrected voltage at the local controller is given by:

$$V_x = V_m \cdot \cos(\omega t + \varphi_{vx} + \varphi_{delay})$$

where, $\varphi_{delay} = 2\pi \cdot f_g \cdot T_{delay}$

T_{delay} is estimated by taking difference of GPS time stamping at sending end (central controller) and receiving end (local controller).

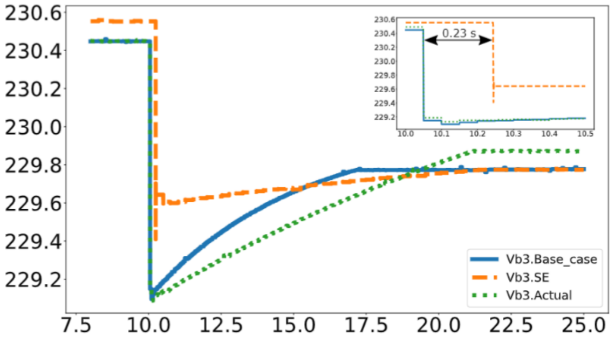


Figure 3: Voltage profile for bus 3

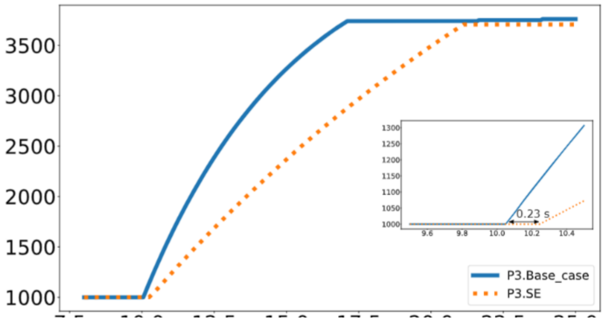


Figure 4: Bus 3 inverter active power dynamic response

Techno-economic analysis of intercontinental electricity grids with future European energy system

Thushara Addanki[a], Thomas Hamacher[b]

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To achieve a carbon-neutral energy system, a single solution often falls short in realizing their purpose due to various economical, technical, and environmental side-effects. The only effective solution is to explore number of different options which can work together. One such option is expansion of transmission grids to carry electrical energy directly through longer distances. This would give the system stability due to the interaction of various generation technologies at various sites, which are sometimes in different time-zones. Though super-grids are not a new idea and were discussed for decades in research [1] with no successful implementation at large-scale, there has been an ever-increasing dependency on HVDC cable technology, which makes this option not obsolete. Such development is also evident in submarine cable technology with more cables being built every year.

The goal of this research is to analyze few intercontinental grids and to investigate the extent to which they bring economic benefit in a fully renewable world with Europe as the focus. The connections between Europe - North Africa, Europe - Middle East, and Europe - Canada are studied. For this purpose, an existing country-level model of European energy system within the framework of linear optimization model *urbs* [2] is used. Extensive research has been done to create simple electricity models of the other world regions. The models are complete electricity models with an hourly temporal resolution. Each country in these models have given a possibility to exchange electricity generation with all its neighboring countries. The Europe – Canada model was created as bridges with Iceland and Greenland in between.

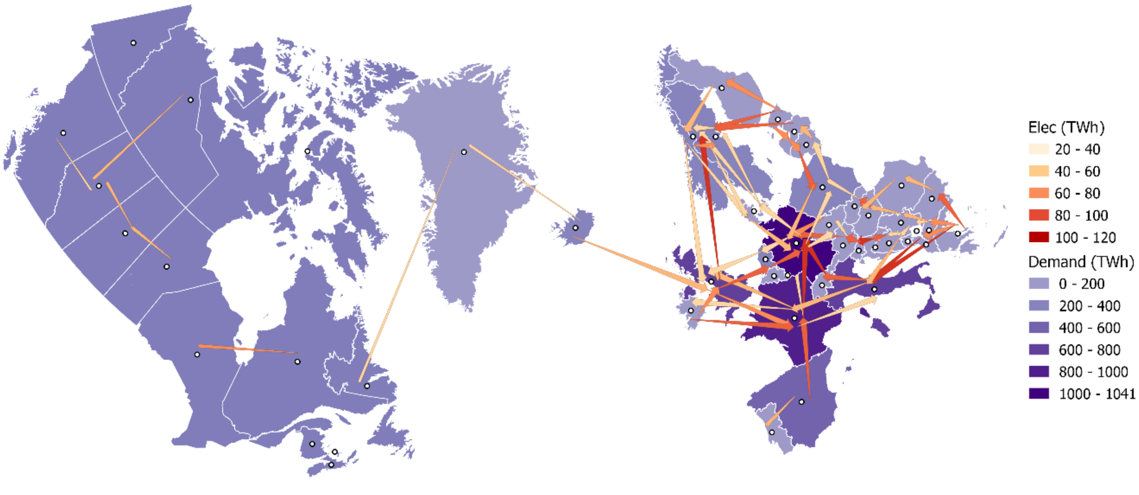

Figure 1: Exemplary Result of Europe – Canada – 2050 model with a limit on transmission capacity to 24 GW per line

Several scenarios are simulated to observe the change in site-selection for generation expansion and the change in the capacity and usage of transmission lines. The first results of this research showed that the imports from PV expansion in North Africa and Wind energy expansion in Iceland would be very profitable for renewable Europe.

References

[1] Trieb, F., Trans-Mediterranean interconnection for concentrating solar power (TRANS-CSP). German Aerospace Center (DLR) Institute of Technical Thermodynamics Section Systems Analysis and Technology Assessment, 2006.

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In situ investigation of thermoelectric thin films based on ionic liquid post-treated PEDOT:PSS

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When opening the newspapers in the past months one gets overwhelmed with articles about energy political issues, increasing energy prices and challenges in energy supply reliability. In this context, but also to sustainably face the constant increasing energy demand in long-term perspective, the need for renewable energy sources is undeniable. Furthermore, as around 50 % of the overall global input energy is accounted for heat loss, energy that dissipates unused into the environment, the topic of waste heat recovery is of immense importance.[1] For this, thermoelectric (TE) generators are of great interest, as they enable the conversion of a temperature gradient directly into electrical power (Figure 1). In particular, TE generators based on polymers are very advantageous, as these usually low or non-toxic organic materials allow a large scale and low-cost solution based processing like printing, dip or spray coating. This facilitates the fabrication of lightweight and flexible TE devices opening a wide range of application.

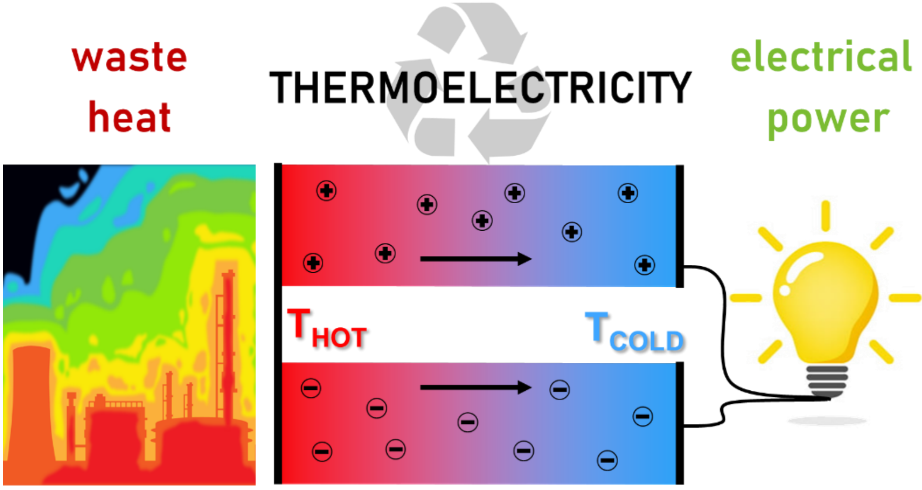

Figure 1: Schematic waste heat recovery with a thermoelectric generator

A remarkable and widely researched organic TE material is the p-type semiconductor poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS). In our studies we use this water-soluble PEDOT:PSS to prepare thin and transparent TE films, and post-treat them in order to enhance their TE properties. Hereby it was found that a post-treatment with ionic liquids (ILs) to be highly effective. By using different investigation techniques, we revealed that this ILs post-treatment affects the morphology and the doping level of our PEDOT:PSS thin films, and therefore simultaneously increases two important TE parameters, the Seebeck coefficient (S) and the electric conductivity (σ).[2]

However, to make these PEDOT:PSS thin films usable in future commercial TE devices it is indispensable to also investigate the performance of these materials for their long-term stability under different ambient conditions, like elevated temperature or increased humidity. Therefore, we performed in situ experiments using a custom-built measurement chamber in which we can heat the ILs post-treated PEDOT:PSS thin films to different temperatures or expose them to a certain humidity, while simultaneously measuring their TE properties.[3] These studies give an important insight and understanding about the impact of respective operation environments for future PEDOT:PSS based TE devices in terms of long term stability.

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Non-uniform lithium distribution in 18650-type lithium-ion battery during dis-/charging

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Lithium-ion batteries play an important role for energy storage in modern society, where they serve as energy sources in portable electronics, like laptops and smartphones as well as in electric vehicles. Their high energy and power density enable a full dis-/charge time in the range of hours meeting typical requirements of daily use. Therefore, lithium-ion batteries and further optimization of their properties are main topics of current research in the field of energy materials and energy storage systems.

Major focus is made on the degradation mechanisms, which in their vary result in a capacity and power fade of the batteries, which is reflected in a loss of active lithium, loss of active electrode material, drift of stoichiometric composition, an increasing impedance of the cells etc [1]. These aging processes inside the cell are determined by a variety of internal and external cell parameters like current density, temperature, etc. These parameters are in general not uniformly distributed throughout the cell. Therefore, degradation rate and state-of-health are inhomogeneously distributed throughout the electrode. Amount of intercalated lithium in the graphite anode can be quantified using diffraction-based techniques. Recent *in-situ* powder diffraction studies on differently aged 18650-type lithium-ion batteries displayed a creation and enhancement of gradients in the lithium distribution in the fully charged graphite anode [2,3].

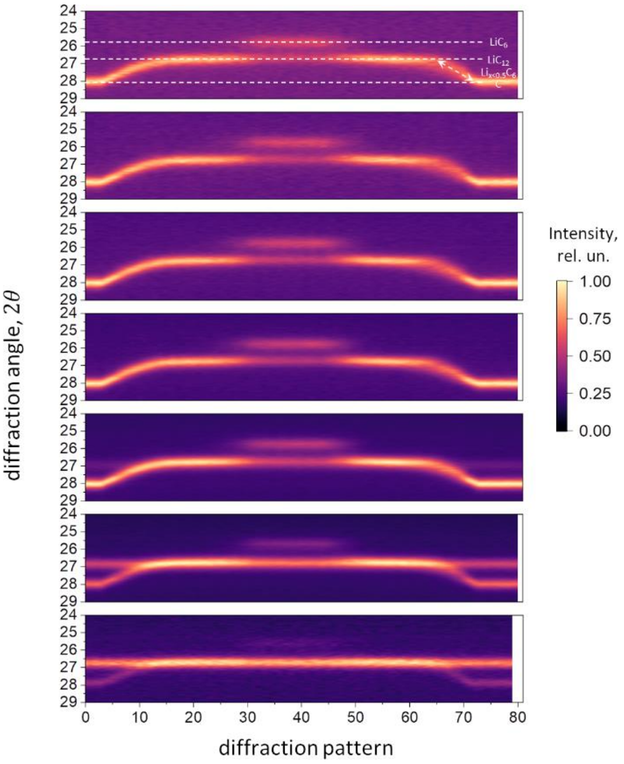

Figure1 False color representation of the scattering intensity resulting from lithiated graphite's of the different gauge volumes in a 18650-type lithium-ion battery. (adopted from Fig. S2 in [4])

In the current work the dynamics of the lithium content in the graphite anode during its de-/lithiation was studied. The lithium concentration was probed using *operando* spatially-resolved neutron powder diffraction while dis-/charging the cell. Set of diffraction patterns were obtained at different areas/regions of the cell (see Fig.1), which enabled a reconstruction of the in-plane lithium distribution during dis-/charging. Diffraction experiments using high-energy photon beams (synchrotron radiation) were performed to complement neutron data in order to get a full picture of the lithium inhomogeneities and their dynamics on different length scales, i.e. on cell and electrode level.

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Manufacturing of new uranium fuel for FRM II conversion

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Nuclear energy represents a main alternative to produce carbonless electricity thanks to fission reaction involved in nuclear plants. In parallel, research reactors were developed since 1942 [1] in order to use directly neutrons provided for many applications in material science, medical sector or fundamental researches as the Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II, Garching, Germany) does since 2005 [2].

Fuel arrays for nuclear power plants differ from research ones in a number of ways: both uranium enrichment & alloy used and geometry. Firsts mainly consist of a stainless steel grid housing Zircalloy rods, filled with UO_2 or MOx (a mix of PuO_2 & UO_2) ceramic pellets typically enriched up to 4% of fissile uranium, ^{235}U [3]. On the other hand, research reactors are generally fueled with metallic uranium-alloy dispersed in an Al powder with enrichments from 20% to 93%. Among those the high-performance reactors (HPRR), FRM II needs 93 % enrichment fuel [1,2]. The latter has a single compact core as an annular tube shape housing 113 involute plates (Figure 1) [2]. The fuel meat is composed of an Al & U_3Si_2 mixture powder cladded by an Al alloy.

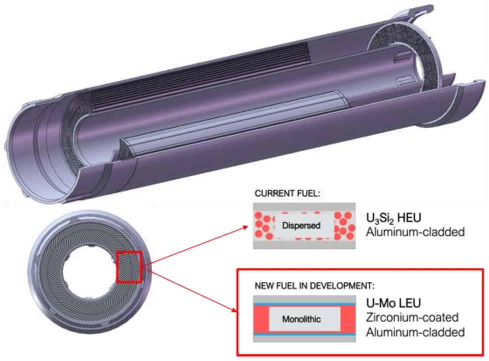

Figure 1: FRM II fuel composition

Within the worldwide effort and framework of the conversion of HPRRs to reduce HEU proliferation, and in the scope of the European HERACLES initiative, FRM II aims to convert its HEU fuel to a lower enriched. To compensate for the loss in enrichment high density metallic fuels are needed. Among uranium alloys, one of the most promising candidates is a monolithic uranium-molybdenum alloy fuel (U-10Mo) with a uranium density up to 15.3 $g.cm^{-3}$ for U-10Mo, considerably higher than actual dispersed U_3Si_2 with 3.0 $g.cm^{-3}$ [2,4]. These metallic high-density fuels are also potential candidates for the fuel of small modular reactors, currently world-wide in development as alternative to the existing generation 3 nuclear power plants.

FRM II works with Framatome-CERCA™ (Romans-sur-Isère, France) to develop a European manufacturing pilot line for the monolithic U-Mo fuel production. The plate will be composed of a U-Mo core coated with few μm thick zirconium (Zr) and then cladded in an aluminum frame. The fuel plate manufacturing follows different steps to obtain the desired properties. After arc and induction casting of raw materials to obtain ingots, these are encapsulated into stainless steel canisters by laser welding. This assembly process is followed by hot rolling to reduce ingot thickness prior to U-Mo bare foil decanning. A step of cold rolling is implemented to finalize characteristics for following process of Zr-coating and Al cladding. Laser cutting process is then realized to adjust foils according to required dimensions while removing some defects. This paper attempts to show mechanical, material science & manufacturing aspects about U-Mo foil production for FRM II conversion. Experiments conducted to understand manufacturing process will be presented in order to produce lowest enriched uranium fuel for research reactors.

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Insights into Current and Future Experimental Investigation of Conventional and Plasma-Assisted Solid Fuel Entrained Flow Gasification

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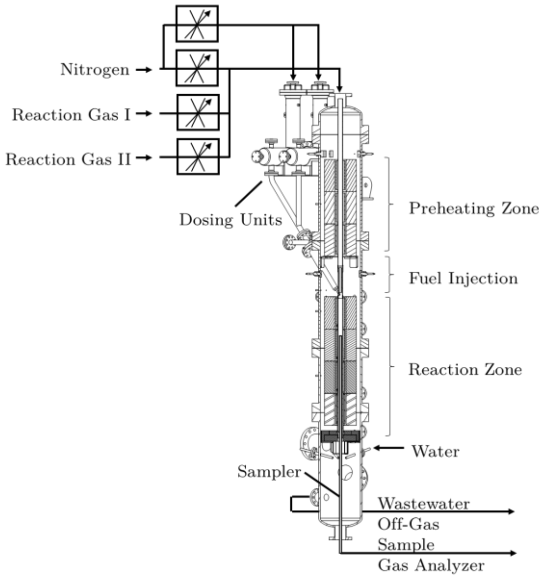

Figure 1: Electrical Heated Gasifier

The Chair of Energy Systems at the Technical University of Munich has a long ranging experience in the investigation of solid fuel conversion under entrained flow conditions. This is mainly due to the *BMWK*-funded project *HotVeGas*, which aimed to investigate the gasification behaviour of different fuel types ranging from fossil fuels to pretreated biomasses and residues. The investigations have mainly been performed in an electrical heated pressurized entrained flow reactor as shown in Figure 1, which can withstand pressures up to 50 bars and temperatures up to 1800 °C. It allows the collection of chars from devolatilisation or gasification experiments under industrial scale entrained flow conditions. The same applies to an autothermal pilot scale gasifier, which is shown in Figure 2. This reactor partially oxidizes fuel with a maximum input of up to 120 KW. In terms of the project, the chars of both reactors have been analyzed in the lab to determine conversions, structural properties and their rates with different gasification agents within thermogravimetric analyzers. The resulting data has now been summarized in a comprehensive database, which is available on Mendeley Data [1] and which is described in Fuel [2]. The database does not include the single data points. It rather lists model parameters discribing the measured behaviors and references to appropriate validation data for simulation purpose. Based on the content of the database, this contribution will first give a brief summary of the current research results. It will e.g. explain the experimental methods, present the applied model equations and discuss or compare the resulting data. Thereby, special focus is on thermal deactivation, surface area development and rates with different gasification agents. Based on these insights, an outlook on recent research activities will be given, which focuses on the implementation of a plasma torch into the pilot scale gasifier in terms of the international future lab on green hydrogen technologies *Redefine H2E (BMWF).*

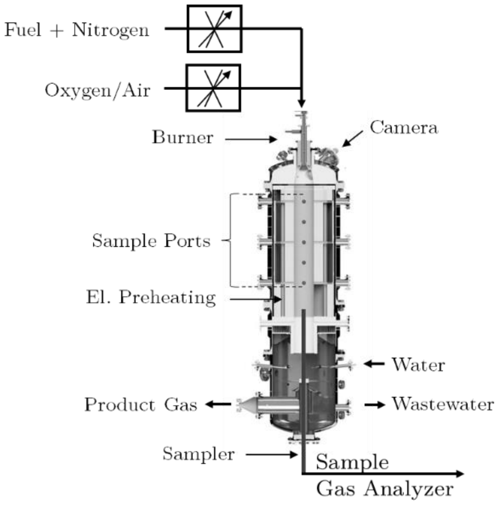

Figure 2: Autothermal Gasifier

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In-Situ Identification of Electrocatalytically Active Areas on Palladium Using Electrochemical Scanning Tunneling Microscopy

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Due to the global aim to reduce climate threatening greenhouse gases, an increasing share of electricity is produced by renewable energy sources in order to replace fossil fuels [1]. Regarding the resulting difficulties for mobile devices, the use of fuel cells poses a viable solution, especially if their costs can be further reduced *e.g.* by using nanostructured electrocatalytic materials on cheap support materials [2]. The active structures which promote electrochemical reactions on electrocatalytic surfaces can be determined by using the noise-Electrochemical Scanning Tunneling Microscopy (n-EC-STM) method. Here, active sites are identified by a higher noise level compared to inactive sites. The noise is caused by the reaction processes within the tunneling gap. Therefore, the local activity of the surface structure can be visualized. The rate of the electrochemical reactions can be controlled by changing an applied potential.[3] The knowledge about the local activity of the decisive structures enables a targeted design of future electrocatalytic materials.

Here, the n-EC-STM method was performed on different Pd single crystals in 0.1M $HClO_4$. The focus in these measurements was set to the hydrogen evolution reaction (HER). As illustrated in Figure 1a, *e.g.* on Pd(111), for the HER turned "On", a high noise and, therefore, activity is found on step edges, while atomically flat areas seem to be less active. However, some steps do not show this increased activity, as visible in the right side of the image. As expected, for the HER switched "Off", the whole noise disappears. This increased noise behavior on steps can also be observed in Figure 1b, quantifying the local activity on the different steps in Figure 1a.

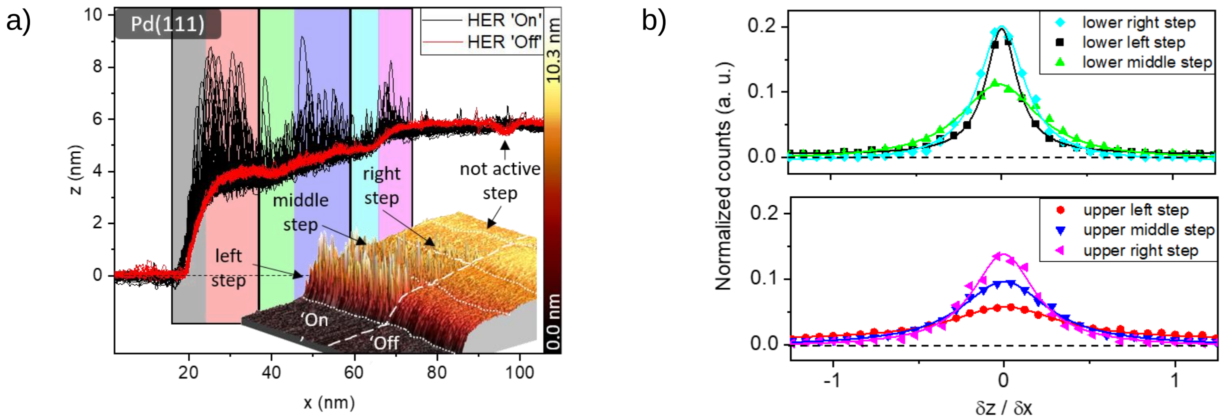

Figure 1. n-EC-STM measurement of Pd(111) in 0.1 M $HClO_4$. a) n-EC-STM measurement for HER switched 'On' and 'Off'. b) Comparison of the HER activity on the lower and upper part of steps with different heights, visible in a. Please note: Both images are already submitted in [4].

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2. Posters

Assessing the Benefit of Optimization Measures for Existing District Heating Systems

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Background

The ongoing research project ‘OREWA’ (Optimization and restructuring of district heating networks including evaluation of transferability, ecology, and economy; Grant number FKZ: 03EN3005) aims to form a generally valid catalog of optimization measures for district heating networks (DHNs). This catalog summarizes published studies and includes the results of ongoing project investigations. In the project, optimization measures for local DHNs are being analyzed using the example of two existing DHNs. The focus is on low-investment measures. These should enable DHN operators to operate their DHNs cost-efficiently in the future.

Objective

There are many studies on optimization measures. However, there is no overview of when which measures are suitable or whether they are useful at all. On that score this contribution presents a method for assessing the benefits of individual optimization measures. Finally, a comparison of the studied optimization measures is performed. The optimization measures were assessed according to their payback period and the final energy savings. These two parameters are used to form a score that allows the various optimization measures to be ranked according to their benefits. This overview represents a decision-making aid for DH operators.

Methodology

The assessing process was carried out in two steps. In the first step, the importance of economic efficiency and ecology was determined using the method of the analytic hierarchy process according to [1]. Experts from the field of energy distribution were asked to assess the importance of a small payback period and high final energy savings when assessing optimization measures. The result of this prioritization was then applied as a point system. For example, an optimization measure with a medium payback period and low final energy savings receives a lower score than an optimization measure with a short payback period and high final energy savings. In the second step of the assessing procedure, the certainty of a prediction about the value of an optimization measure is integrated into the ranking system by means of a weighting factor. If, for example, three studies concluded that a certain measure has been identified as highly effective in terms of economic efficiency and ecology, this measure is assigned a higher score in the ranking than a measure which has been identified as highly effective in one study only. In total, there are three ranges of results. The ranges result from the fact that some optimization measures perform well in all studies (high potential). Other optimization measures have been identified as helpful in some studies but not in others (medium potential). And then there are optimization measures that have been identified as inefficient in all studies (no potential). The ranking thus offers the DH operator a quick orientation aid.

Results

The procedure described in the methodology was successfully implemented. The experts assigned greater importance to economic efficiency than to ecology. This implies that low-investment measures with high or medium final energy savings were given a particularly high prioritization. After analyzing all measures, the distribution of measures according to their potential is roughly as shown in Figure 1. Only few measures were identified as highly effective. The most measures fall into the medium potential category. The share of measures with no potential is greater than the share with high potential.

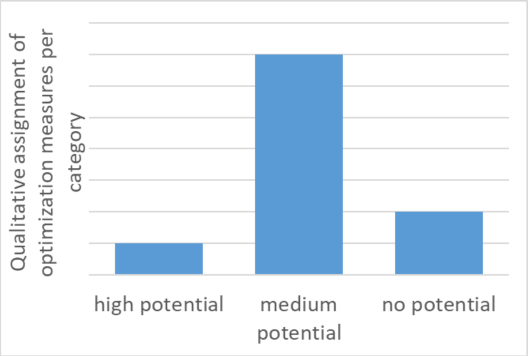

Figure 1 Distribution of optimization measures according to their potential

Conclusion

The method for assessing optimization measures offers an unprecedented possibility, namely an overview of different scientific studies on optimization measures. The catalog of the assessed optimization measures is the basis for the selection of optimization measures in practice. A guide is still being prepared to show DH operators how to work with this catalog.

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Facile and surfactant-free synthesis of Pd/C nanostructured (electro)catalytic materials

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Environmental concerns have prompted the development of cleaner synthetic approaches for supported precious metal nanoparticles (NP) [1]. Control of the size, shape and distribution of the NPs over the support allows for optimal use of noble metals and higher catalytic efficiency [2]. Colloidal synthesis approaches allow for the aforementioned control, but their reliance on surfactants and high boiling point solvents complicates their implementation on an industrial scale. Recently elaborated synthesis routes allow for avoiding these problems; however, without the NPs shape control, which is an important parameter in the design of catalysts [3]. This work suggests a simple, fast and surfactant-free synthesis method to produce carbon supported palladium nanoparticles (Pd/C) at room temperature. In addition to control of the NP size and distribution on the support, this method also allows control of the shape of the Pd NPs. This is at odds with state-of-the-art literature, where using different precursor salts or additives for influencing Pd NP morphologies is suggested [4].

In this work, $PdCl_2$ was reacted with HCl to form H_2PdCl_4 and then dissolved in anhydrous methanol to a concentration of 20 mM. In addition, a second stock solution of 57 mM NaOH in methanol was prepared. Vulcan carbon (VXC72R) was dispersed in the alkaline methanol before adding the Pd solution. Afterward, both stock solutions were mixed and left under vigorous stirring at room temperature for various synthesis durations. Depending on the used volume of each stock solution, the catalysts obtained at different molar ratios of NaOH/Pd were compared. It was found that the molar ratio of NaOH to Pd in the synthesis solution has an influence on the shape of the obtained Pd NPs without changing the precursor salt or using any additives. Moreover, Pd NPs produced with a lower NaOH/Pd molar ratio of 10 display spherical morphologies, while the higher molar ratio (NaOH/Pd = 30) displays the formation of Pd nanodentrite-like structures (Figure 1).

The nanodentritic Pd NPs (~25 nm) produced by this simplified process demonstrate a higher activity towards ORR in acidic media than 6 times smaller spherical Pd/C NPs (4.2 nm) from the literature [5]. More specifically, we have an improvement of up to 4 times of specific activity and up to 2.5 times improvement of mass activity (Figure 2). This shows that Pd also favorably catalyzes ORR in the presence of surface concavities, similarly to platinum [2].

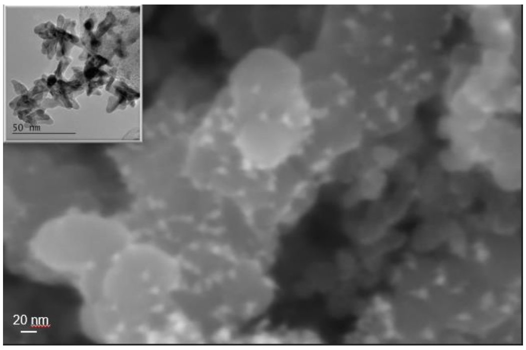

Figure 1: SEM and TEM (Inset) of obtained Pd/C NP

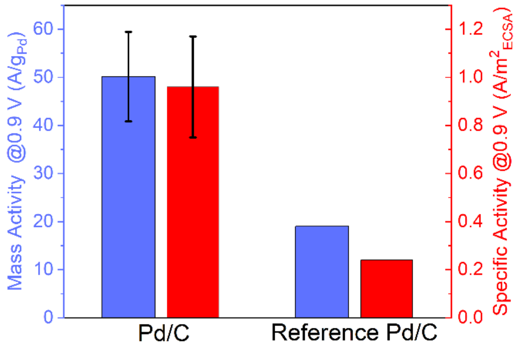

Figure 2: ORR (0.1 $HClO_4$, 1600 rpm) mass activity and specific activity of obtained Pd/C NP and reference catalyst [5]

Acknowledgment: This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement HERMES No 952184. We are thankful to Frederic Maillard and Arnaud Viola for TEM measurements.

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Powder-based Additive Manufacturing of Pt/Al_2O_3 catalysts for LOHC Dehydrogenation

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Conventional catalyst shaping techniques for heterogeneous catalysis include tabletting, extrusion or granulation [1]. Sufficient mass and heat transfer, low pressure loss, short diffusion paths, an adequate pore size distribution or the specific surface area are some of the parameters affected by the macro- and microscale geometric design of a reactor packing. The application of additive manufacturing allows almost unlimited shape variation and has received increased attention during the last decade so that numerous 3D printing techniques have already been put to test for solid catalyst fabrication [2]. In this study, the powder-based Binder Jetting (BJ) technique (Fig. 1) was used to evaluate the fabrication of alumina-based supported Pt catalysts which were tested for the dehydrogenation of the liquid organic hydrogen carrier (LOHC) perhydro-dibenzyltoluene (18H-DBT), a medium for reversible hydrogen storage via catalytic processes.

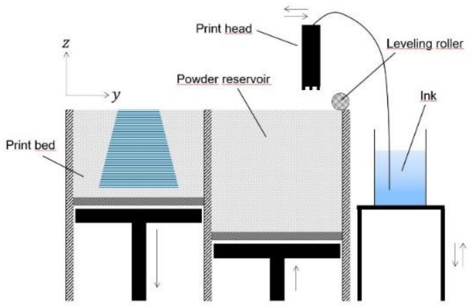

Figure 1: Basic schematic of a Binder Jetting setup.

Monolithic alumina supports and cylindrical test geometries for characterization were fabricated according to a previously reported manufacturing route [3]. Calcination temperature and impregnation time variation experiments were conducted to detect the optimal conditions for application in LOHC dehydrogenation. The pore size distribution (poreSD) was determined via nitrogen gas adsorption (BJH) and mercury intrusion porosimetry (MIP) where a porosity of 77 % was measured. The Pt loading, metal particle size and dispersion were determined via ICP-OES and TEM, respectively. Pt was highly dispersed on the alumina surface with particle diameters as small as 1.10 nm and a maximum dispersion of 91.9 %. Monoliths prepared with a calcination of 1100 °C and an impregnation time of 3 h were chosen for catalytic testing to limit restrictive diffusion of the reactant during dehydrogenation.

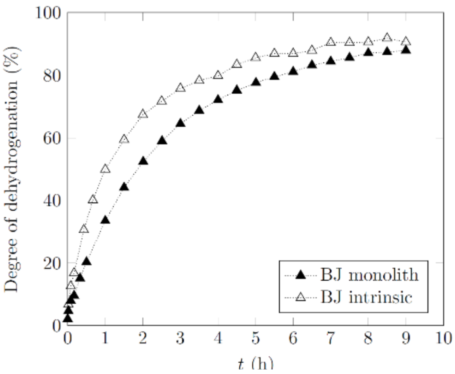

Figure 2: LOHC dehydrogenation over BJ printed Pt/Al_2O_3 catalysts.

The catalytic performance was tested with monolithic catalysts and crushed monoliths for intrinsic tests (Fig. 2). In general, the powder catalyst showed higher dehydrogenation rates due to minimized diffusional limitations. However, the final degree of dehydrogenation for the monolithic and intrinsic tests were similar with 87.9 % and 90.6 %, respectively, showing that powder-based 3D printing provides a viable method to fabricate supported noble metal catalysts for environmental applications such as the dehydrogenation of LOHC with tailor-made catalyst geometries.

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Investigation of the charge transport in ionic liquid post-treated PEDOT:PSS thin films with in-situ impedance spectroscopy

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Waste-heat recovery is an approach to face the climate crisis, by making use of the enormous amount of energy, which would otherwise be lost without being utilized. For this, thermoelectric generators can be used as they offer the possibility to generate electric energy from a temperature gradient. In the past when these devices were developed, they were mainly used for space applications. Nowadays, a big application potential lies in waste-heat harvesting from e.g. combustion engines. Furthermore, the internet-of-things represents another big application field of thermoelectric devices in our future daily life. Here the aim is to power devices, such as watches, mobile phones or sensors using the temperature gradient between, e.g. the skin and the environment and thus reduce the need of a charging process or even make it redundant.[1]

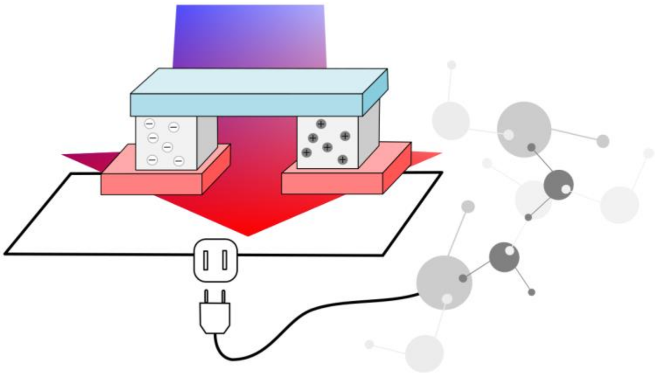

Figure 1: Schematic illustration of a thermoelectric generator under influence of a temperature gradient providing the electric current (DC) for a plug and thus powering certain electric devices.

Our research focuses on optimizing thermoelectric materials based on polymers as they enable large-scale and low cost processability from solution and possess advantageous properties like lightness, non-toxicity and low thermal conductivity. A very promising candidate and centre of our investigation is poly(3,4-ethylene dioxythiophene):poly(styrene sulfonate) (PEDOT:PSS), prepared as a thin film and post-treated with different ionic liquids (ILs), using the spin coating process. PEDOT belongs to the class of conjugated polymers and can be processed from aqueous solution when used as blend with the water-soluble component PSS.[2]

Thermoelectric power supply aims for a constant charge flow, which in this application field can be provided by electric charge carriers, but not by ionic charge carriers. This encourages to investigate the quantity of the ionic Seebeck effect in our thermoelectric materials. Conductivity measurements imply, that the environmental factors temperature and humidity may have a significant impact on the movement of ionic charge carriers, in our ILs treated PEDOT:PSS thin films. For this reason, the approach is to use Galvanostatic Electrochemical Impedance Spectroscopy (GEIS) to determine the electronic and ionic contribution to the thin films conductivity.

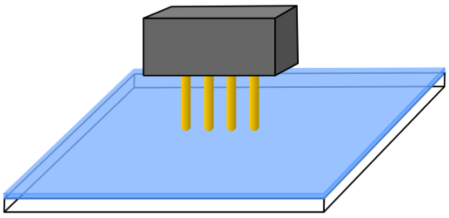

Figure 2: PEDOT:PSS sample contacted by four gold-pins, in order to perform impedance measurements

The gathered better understanding yields the chance to enhance and optimize not only to the manufacturing of PEDOT:PSS thin films for thermoelectric application, but moreover helps to understand the effect ILs have on conjugated polymer based materials.

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In-situ Scanning Tunneling Microcopy Imaging of Active Sites for Electrolyser and Fuel Cell Applications

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With an increased awareness of the severe consequences of climate change, it becomes more pressing than ever that a new way of thinking and research has to develop to drastically reduce our "carbon footprint" on the planet. An important tool to turn around the current trends are electrochemical energy conversion and storage devices such as electrolysers and fuel cells. However, due to their often limited reaction kinetics and lack of suitable catalysts, these devices remain unsuitable for large-scale commercialization. In turn, suitable catalysts are necessary, which rely on smart design principles regarding their material composition, shape and size. Hereby, the knowledge of active sites, at which a reaction is efficiently catalyzed is of paramount importance.

A direct experimental tool to identify active sites is electrochemical scanning tunnelling microscopy (EC-STM), which can achieve nanometer to atomic-scale resolution. If no reaction takes place at the catalyst surface, the STM signal will be stable (Figure 1a). This is also the case during an ongoing reaction if the tip is kept over an inactive site (Figure 1b, grey atoms). However, if the tip moves over an active area, the signal will get noisier (Figure 1b near the step edge). The higher the reaction overpotential, the larger this noise signal will be. This noise signal can then be further analysed. This way it is not only possible to visualise active sites, but also quantitatively analyse them and their reaction kinetics. In the example in Figure 1, active sites are near step edges. This can occur due to a different energetic structure and therefore better adsorption or desorption parameters for the specific chemical reactants and intermediates. This example holds for Pt(111) surfaces and the oxygen reduction reaction[2].

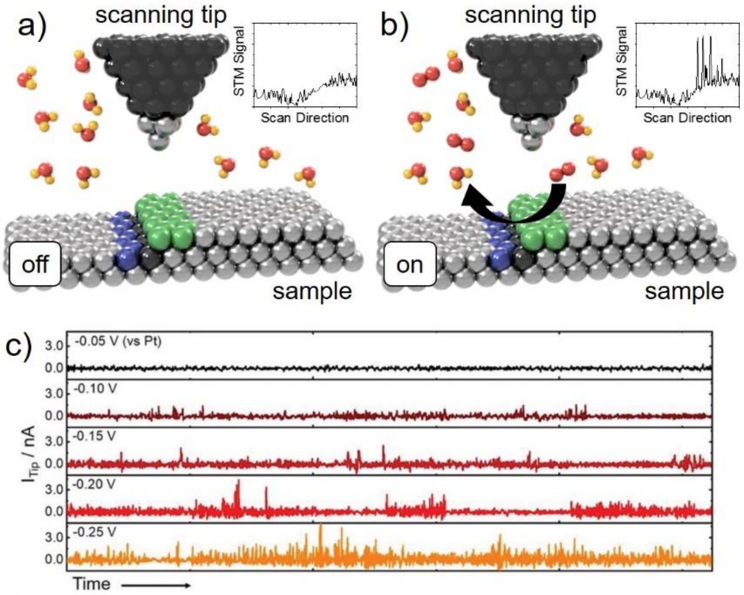

Figure 1. A schematic overview of the in-situ detection of active sites using an EC-STM. The electrochemical reaction can either be switched "off" or "on" by the application of a suitable potential. a) In the "off" state, no reaction occurs and the tunnelling current remains rather constant. b) If the reaction is switched "on", a noise develops at the active sites (here, near the step edge). c) The extent of the noise dependents on the selected overpotential. Here, the oxygen reduction reaction on Pt(111) is shown as example. The images a,b) are reprinted with permission from reference [1], and c) from reference [2] © 2020 The Authors. Published by Wiley-VCH GmbH.

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Inorganic-organic hybrid nanostructures based on biopolymer templating

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Inorganic-organic hybrid nanostructures are researched for many different applications. This work is focused on energy conversion through the thermoelectric effect. With the Seebeck effect, electrical current can be generated from a temperature difference. Therefore, thermoelectric generators could be used to generate energy from waste heat. As waste heat is abundant in almost all energy applications, thermoelectric elements could save large amounts of energy in many different areas of technology.

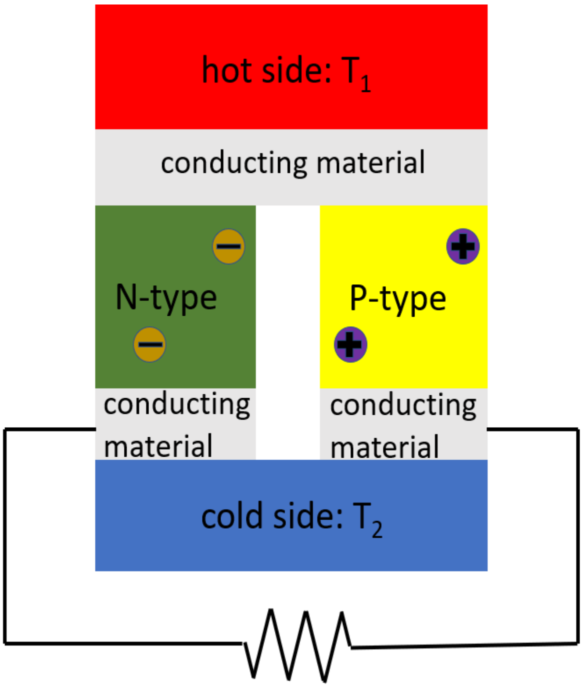

Figure 1: Thermoelectric circuit composed of an n-doped and a p-doped material. (different Seebeck coefficients)

However, the current thermoelectric generators (TEG) often use materials like bismuth (Bi), tellurium (Te), antimony (Sb) or lead (Pb). These materials are toxic and expensive giving rise to a need for a cleaner and more abundant alternative that still produces good conversion efficiencies.

The efficiency of materials to produce thermoelectric power is mainly governed by three factors. The Seebeck coefficient (S), the electrical conductivity (σ) and the thermal conductivity (κ). Increasing S and σ while decreasing κ would lead to an increased performance. Nanostructuring can help tune these parameters. For example, encapsulating air can help decrease thermal conductivity, while a sufficient percolation network can increase electrical conductivity.

Beta-lactoglobulin is a bovine whey protein, that is known to form different aggregates under different environmental conditions. By changing the pH-value and protein concentration, different morphologies can be achieved. Therefore, beta-lactoglobulin is used to structure titania (TiO_2) using sol-gel synthesis with water as the solvent. Slot-die coating is used to enable industrial mass-production.

The differently structured beta-lactoglobulin-titania thin-films are studied with AFM and SEM imaging. With these measurements the morphology of the samples can be investigated. Seebeck coefficient and electrical conductivity of the samples are measured using a 4-point probe setup. From this the thermoelectric Figure of merit (zT) can be calculated and compared with the different sample morphologies. The structure formation during printing is investigated in real time, using in situ GISAXS measurements. From this, time-resolved information about average domain sizes and domain distances can be obtained.

CO_2 Plume Geothermal (CPG) Systems for Combined Heat and Power Generation

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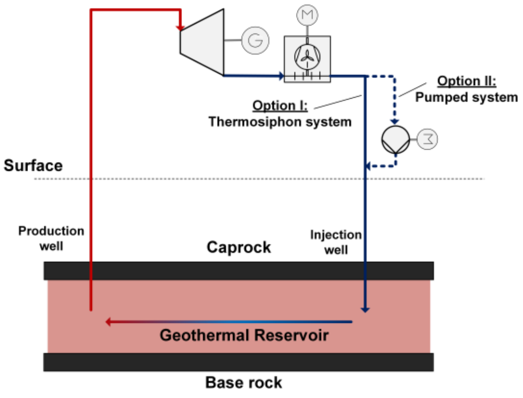
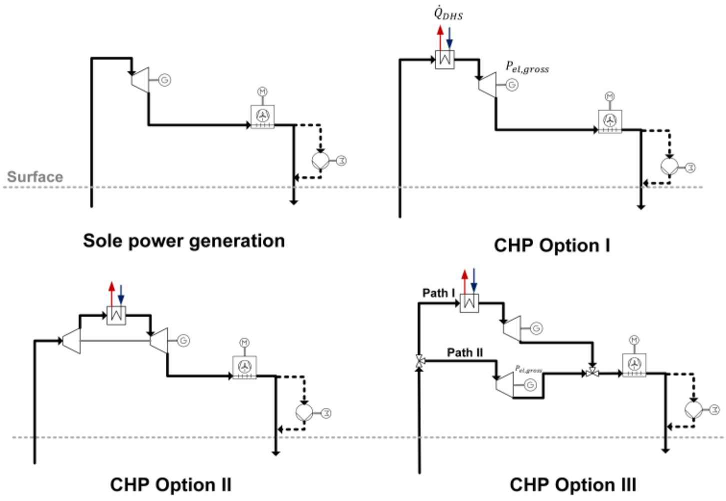


Figure 1: Genearal concept of a CPG system

Petrothermal geothermal energy has a tremendous worldwide potential for decarbonizing both the power and heating sector [1]. While the conventional utilization concept foresees the use of water as a heat carrier, CO_2 might be a promising alternative heat carrier, due to several potential advantages. Because of the high density differences of the CO_2 between the cold injection and hot production well (cf. Figure 1), the CO_2 circulates without the need of an additional pump through the reservoir - the so-called thermosiphon effect [2]. Additionally, the CO_2 can be used directly in a turbine for power generation even at low reservoir depths [3]. Finally, such so-called CO_2 plume geothermal (CPG) systems are an attractive concept for utilizing petrothermal resources in the context of a future carbon capture utilization and sequestration economy. This work investigates three potential CPG configurations for combined heating and power generation (CHP): (i) a serial configuration with the heat exchanger for the district heating network (DHS) before the turbine; (ii) a two-staged serial configuration with the DHS supply on an intermediate pressure level and (iii) a parallel-serial configuration [4]. The different configurations are visualized in Figure 2. The different configurations are evaluated for various scenarios with reservoir depths of 4 and 5 km, and required DHS supply temperatures of 70 and 90 °C. The results reveal that a two-staged serial CHP concept eventuates in the highest achievable net power output. For a thermosiphon system, the relative net power reduction by the CHP option is significantly lower than for a pumped system. The net power reduction for pumped systems lies between 62.6 and 22.9 %. For a thermosiphon system with a depth of 5 km and a required DHS supply temperature of 70 °C, the achievable net power by the most beneficial CHP option is even 9.2 % higher than with sole power generation. The evaluation of the achievable revenues demonstrate that a CHP application might improve the economic performance of both thermosiphon and pumped CPG systems. However, the minimum heat revenue required for compensating the power reduction increases with higher electricity revenues. In summary, the results of this work provide valuable insights for the potential development of CPG systems for CHP applications and for the assessment of their economic feasibility.



Sole power generation

CHP Option I

CHP Option II

CHP Option III

Figure 2: Visualization of the reference scenario for sole power generation and the three investigated CHP configurations.

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Impact of CO_2 activation on structure, composition, and performance of Sb/C nanohybrid lithium/ sodium-ion battery anodes

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Antimony (Sb) has been regarded as one of the most promising anode materials for both lithium-ion batteries (LIBs) and sodium-ion batteries (SIBs) and attracted much attention in recent years.[1] How to alleviate the volumetric effect of antimony during change and discharge processes is the key point to promote Sb-based anodes to practical applications. Carbon dioxide (CO_2) activation is applied to improve rate performance of the Sb/C nanohybrid anodes caused by limited diffusion of Li/Na ions in excessive carbon component.[2] Based on the reaction between CO_2 and carbon, CO_2 activation can not only reduce the excess carbon content of the Sb/C nanohybrid but also create abundant mesopores inside of the carbon matrix, leading to an enhanced rate performance. Additionally, CO_2 activation is also a fast and facile method which can perfectly adapt to the fabrication system. As a result, after CO_2 activation, the average capacity of the Sb/C nanohybrid LIB anodes is increased by about 18 times (from 9 mAh g^{-1} to 160 mAh g^{-1}) at a current density of 3300 mA g^{-1}. Moreover, the application of the CO_2-activated Sb/C nanohybrid as sodium-ion battery anode is also demonstrated, showing a good electrochemical performance.

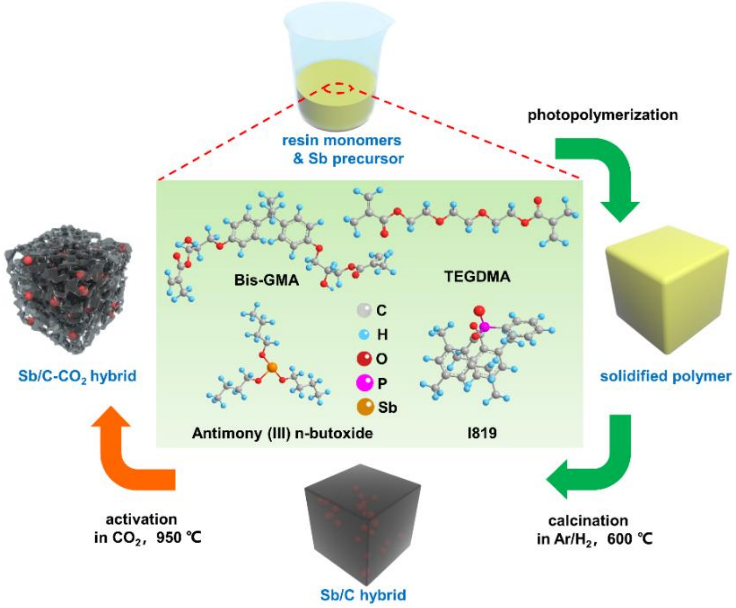

Figure 1: Schematic illustration of the preparation process of the Sb-based nanohybrids without CO_2 activation (Sb/C hybrid) and with CO_2 activation (Sb/C-CO_2 hybrid)

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Influence of Solvent and Lithium Salt on the Structure and Performance of NCM111 Cathode for Lithium Ion Batteries

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Lithium ion batteries (LIBs) with a wide range of applications have emerged as the most promising candidate for electrochemical energy storage due to its higher specific energies, volumetricenergy densities and power densities. As shown in Figure 1, during charge and discharge process, Li^+ shuttles between two electrodes, meanwhile, lithium dendrite will growth and the Coulombic efficiency (CE) will decrease with Li plating and stripping [1]. The abovementioned problems could hinder the serve life and stability of LIBs, and can be ascribed to the increased inhomogeneity and stress at the electrode/electrolyte interface during cycling.

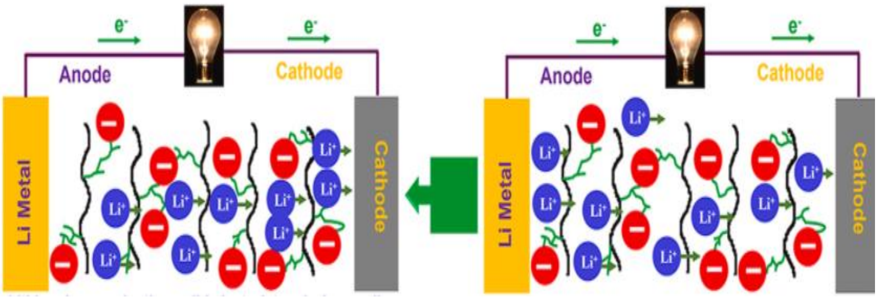

Figure 1: Working principle of lithium ion batteries.

To fulfill the high demands on long serve life and stable LIBs, more and more state-of-art materials has been explored such as $LiNi_{0.9}Mn_{0.05}Co_{0.05}O_2$ for cathode materials [2]. Nevertheless, fundamental research on the component composition and the effect of additive and solvent on LIBs is still lacking. It is of great value to get a deep understanding and therefore optimize the fabrication process for future studies on the electrode/electrolyte interface of LIBs.

In this project, we select the $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ as cathode material to find out the effect of different solvents and extra lithium salt (LiTFSI) on the performance of LIBs. The Li/cathode cells were assembled to observe the battery performance and grazing incidence wide-angle X-ray scattering (GIWAXS) technique is used to detect structure change within the cathode before and after cycling.

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Operando study of light and moisture induced degradation of perovskite solar cells

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Perovskite solar cells (PSCs) are one of the most promising photovoltaic technologies and reached a certified 25.5% efficiency owing to their tunable bandgap, high carrier mobility, long diffusion length and so on.[1] The long-term operational stability of PSCs, however, has been not investigated. Herein, we probe the structure change with grazing-incidence small-angle scattering techniques (GISAXS) under 1-sun illumination and high humidity. Also, the solar cell parameters are obtained simultaneously during the device operation. We find that PSCs fabricated with and without cesium iodide (CsI) show differences in the device degradation and morphology change in the perovskite layer. The decrease of open-circuit voltage (V_{OC}) can be attributed to the morphology changes and the evolution of crystallize grain size. With the additive of CsI, solar cells show slow decay of V_{OC}, which is correlated to improved morphology of active layer and passivation of trap states. Our work presents a crucial step towards a fundamental understanding of morphology change combined with solar cell parameters during the device operation.

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Stacking Kinetics of PbS QDs Orientated by Perovskite Matrix during Slot-Die Printing

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PbS colloidal quantum dots (CQDs) have generated great interests in various optoelectronic devices including solar cells, photodetectors and infrared light-emitting diodes (LEDs), due to their size-tunable bandgap, low-temperature and solution processability. To date, defects and carrier transport in CQD solids and surface passivation of one single QD remain major challenges for the performance of QD based devices. Perovskite matrix or shelling mixed in QDs solution, as one of strategies to solve these issues, is able to provides long diffusion length and serves as excellent passivation for QDs film by the growth of epitaxial interface with good quality. Meanwhile, the solution ligand exchange used in this strategy and solution processibility of QDs and perovskite allow the one-step deposition of QDs active layer, which offers great potentials for large-scale production of QD based optoelectronic devices.

Based on these literatures[1–3], we apply PbI_2, methylammonium (MAI) and perovskite precursors composed of PbI_2 and MAI as the ligand precursors to conduct solution ligand exchange for as-synthesized PbS QDs, and the final QD powder is dissolved with n-butylamine to obtain QD ink for slot-die printing. In this work, we focus on how QDs capped with different ligands dynamically stack in the phase transition from QDs ink to a film during slot-die printing by grazing-incidence small-angle X-ray scattering (GISAXS). In addition, the post-treatment annealing and heated substrate during the film deposition are respectively investigated to observe the inner structure of QDs film in real time. Meanwhile, grazing-incidence wide-angle X-ray scattering (GIWAXS) and GISAXS are simultaneously used to investigate how the perovskite ligands form into crystals and how the crystalline orientation of perovskite matrix dynamically aligns and influences the QDs stacking behavior in the final film formation.

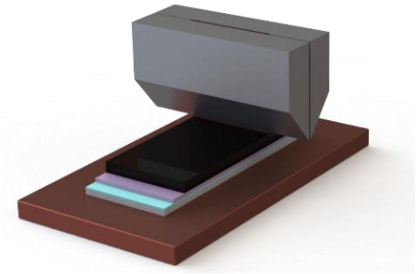

Figure 1: Slot-die coater

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Simultaneously Enhanced Performance and Stability of NFA Solar Cells with PETMP Interfacial Process

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Organic solar cells have called high research attention due to their various advantages and rapid development in recent years. The PCE of non-fullerene acceptor (NFA) solar cells has reached over 19%,[1] while the limited illumination stability is still a big bottleneck before real application. For NFA solar cells, the degradation at ZnO/BHJ interface under illumination is proved to be one of the key sources for performance decrease. It was reported that the hydroxyl radicals of ZnO forming under illumination would cause the degradation of the acceptor material. They could be effectively suppressed through modifying ZnO with a radical trapping agent, of which 2-phenylethylmercaptan (PET) showed the best effect.[2] Unfortunately, PET is highly toxic with a bad smell, which is not acceptable for industry.

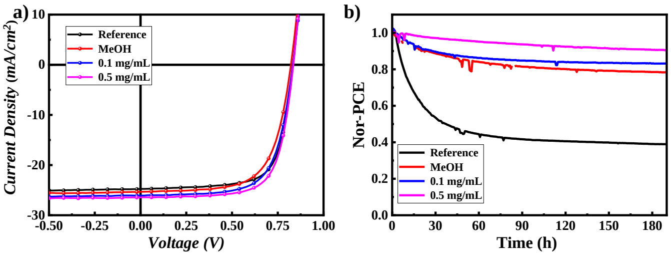

Figure 1: J-V curves and b) Normalized PCE degradation curves of PM6:Y6 devices modified with PETMP

Here, a molecule with similar end group as PET, namely PETMP, is used as the alternative since it has four sulfhydryl groups in one molecule. Fig 1a shows the J-V curves of PM6:Y6 devices modified with different concentration of PETMP, from which we can see that the J_{SC} of the devices increased gradually with higher concentration, while too much PETMP would cause a poor FF due to the interfacial barrier. Then the devices were put under illumination and Fig 1b demonstrates the PCE changes with time. It can be seen that MeOH could improve the device stability greatly since it's a hygroxyl radiation trapper agent as well as reported. Interestingly, PETMP is able to further suppress the interfacial degradation and slow down the performance decay. Such a modification effect is quite similar with that of PET as reported before, suggesting the same function of PETMP here.

Furthermore, the modification effect of other sulfhydryl derivatives was investigated. Fig 2a shows the J-V curves of PM6:Y6 devices modified with different sulfhydryl derivatives, where only modification with more sulfydryls could improve the J_{SC} as well as PCE. Fig 2b and c demonstrate the UV-vis absorption spectra of ZnO films and PM6:Y6 films on ZnO. The improved absorption of ZnO films after interfacial modification may cause the difference in device performance (especially FF). The relatively enhanced signal of Y6 in blend films may be related to the improvement of J_{SC}.

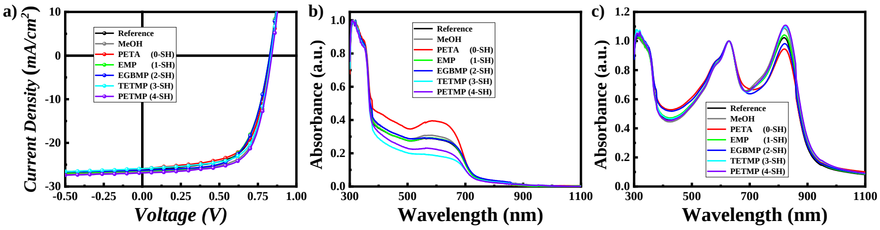

Figure 2: a) J-V curves of PM6:Y6 devices modified with different sulfhydryl derivatives, UV-vis absorption spectra of b) ZnO modified with different sulfhydryl derivatives and c) PM6:Y6 films on ZnO modified with different sulfhydryl derivatives.

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High-concentration Lithium-ion Electrolyte Overcomes the Challenges of High-temperature Lithium Batteries

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Lithium metal battery has been regarded as the “holy grail” for next generation energy storage systems because of its high theoretical specific capacity (3860 mAh/g) and low electrode potential (-3.04 V vs. standard hydrogen electrode). [1] [2] Traditional Li-ion batteries, on the other hand, are severely constrained in high-temperature applications due to the low thermal stability of the electrolyte/electrode interface and electrolyte decompositions in the cell. [3]

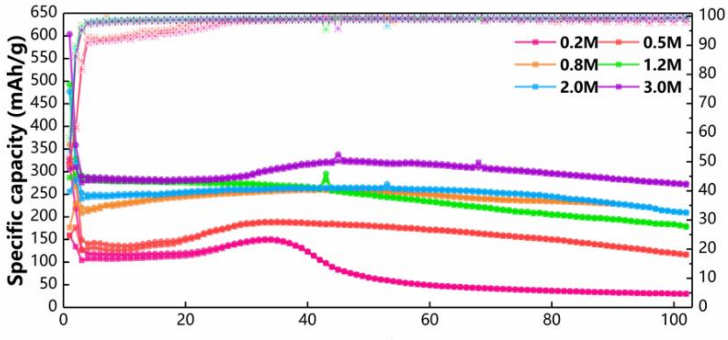

Figure 1 The long-term performance of MCMB/Li at 100 °C

Herein, we have demonstrated a new electrolyte that achieved an excellent stable long-term cycling at 100 °C, well beyond the typical 60 °C limits of normal conventional Li-ion batteries. The high concentrated lithium oxalyldifluoroborate (LiODFB) was selected as the only lithium salt with a carefully designed high thermal stability solvent group. As a result, this unique high-concentration electrolyte can promote to form a stable and inorganic solid electrolyte interface (SEI) layer on the electrode at elevated temperature, leading to improved performance in MCMB/Li and lithium iron phosphate (LFP)/Li half-cells, and achieved reversible capacities of 160 and 350 mA h/g, respectively, with Coulombic efficiencies (CEs) >99.3 % as shown by **Fig 1**.

Subsequently, we further investigate the mechanism of high concentration LiODFB electrolytes by XPS characterization techniques. **Fig 2** shows the component of the SEI formed in high-temperature with different concentration electrolytes, suggesting that the SEI layer consisted of more inorganic compounds, meaning that high-concentrated LiODFB electrolyte promotes the more inorganic SEI film to improve the stability of Lithium metal batteries in high temperature.

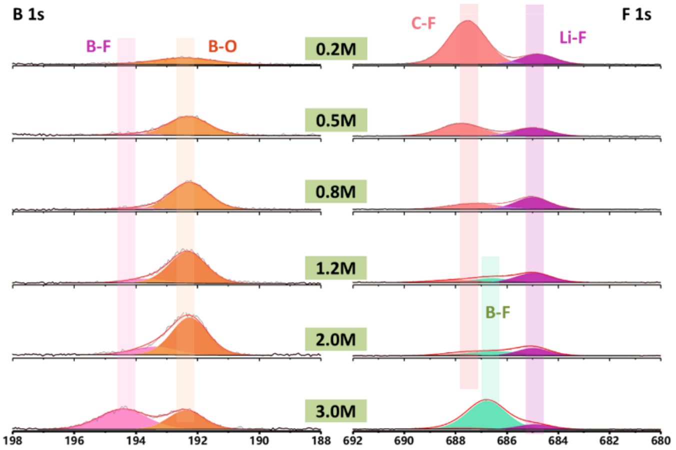

Figure 2 The XPS data of B 1s and F 1s after 100 cycles in different electrolytes

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Design, fabrication and nano-scale characterization of novel SEI layers

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Lithium (Li) has a high specific capacity of 3860 mAh g^{-1} and a low electrochemical potential (-3.04 V), promising a high energy density lithium metal battery (LMB). However, the growth of lithium dendrites during charging and discharging would penetrate the separators in LMBs, which leads to short circuit or even fire, thus causing serious safety problems of LMBs. To inhibit the growth of lithium dendrites and significantly improve the safety of LMBs, the solid electrolyte interphase (SEI) layer is of growing interest. Different methods for the optimization of adjusting mechanical and electrical properties of the SEI layer, including regulating the composition of the electrolyte, the composition of the interface and the morphology, were reported.

In the present work, we focus on optimizing the SEI layer for high specific energy LMBs through localized iodination for an interface and ion modulation.

In the standard electrolyte (PC (propylene carbonate)/FEC (fluoroethylene carbonate)/DMC (dimethyl carbonate)=7.5/2/0.5 v/v/v, 1.05 M LiTFSI (lithium bis(trifluoromethanesulfonyl)imide), a small amount of additive (poly (N- vinylimidazole) quaternized with iodide, molecular weight 16.5 g/mol, 21% quaternization, abbreviated as PVIM) was added. As shown in Figure 1, the Li-Li symmetrical cells with the PVIM additive electrolyte can cycle for 200 cycles under the charge/discharge conditions with a capacity setting of 1 mAh cm^{-2} (red curve) and a current density of 2 mA cm^{-2}, while the control sample can only cycle for nearly 100 cycles (black curve). On the one hand, PVIM releases iodine ions during the dissolution process, which can effectively improve the ionic conductivity of the electrolyte. In addition, iodine ions can spontaneously form I^{3-}, which can react with dead lithium, inhibit the formation of lithium dendrites and increase the efficiency of lithium utilization. On the other hand, the nitrogen-containing functional group in the imidazole group can form a solid electrolyte layer with high ionic conductivity, which inhibits the formation of lithium dendrites.

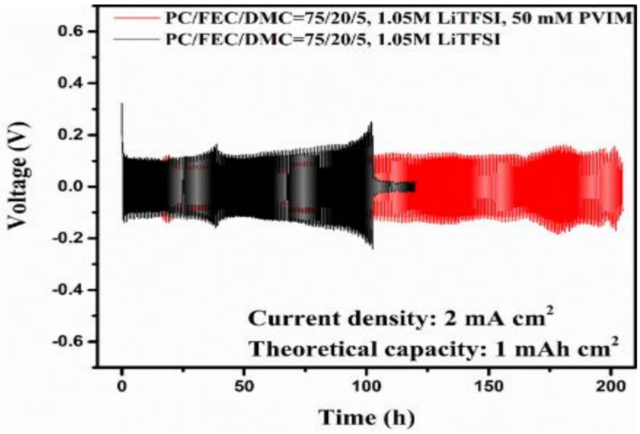

Figure 1: Plating/exfoliation process of lithium/lithium symmetrical cells in two electrolytes: with PVIM electrolyte additive (red) and without electrolyte additive (black) with a capacity setting of 1 mAh cm^{-2} and a current density of 2 mA cm^{-2}.

Role of Unreacted/Excess PbI_2 on the Degradation of Perovskite Solar Cells

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Hybrid organic-inorganic lead halide perovskite materials have attracted tremendous interest over the past few years as its excellent photovoltaic properties in perovskite solar cells (PSCs) with record power conversion efficiency. Unreacted/excess lead iodide (PbI_2) has been universally used in the state-of-the-art devices to boost the device performance. However, the role of unreacted/excess PbI_2 on the degradation of PSCs has not been fully understood and, therefore, needs to be deeply investigated for further improvement of device performance. Herein, it is shown that PbI_2 is unstable under continuous light radiation. The photodecomposition products (lead and iodine) of PbI_2 pose a threat to the efficiency and stability of devices. Thus, unstable PbI_2 under light radiation is one of the main reasons for the degradation of perovskite device. Therefore, carefully controlling or eliminating the unreacted/excess PbI_2 in perovskite film is one of the critical methods to improve the long-term stability of PSCs.

Effect of ionic liquids on crystallization, charge carrier dynamics and stability of perovskite solar cells

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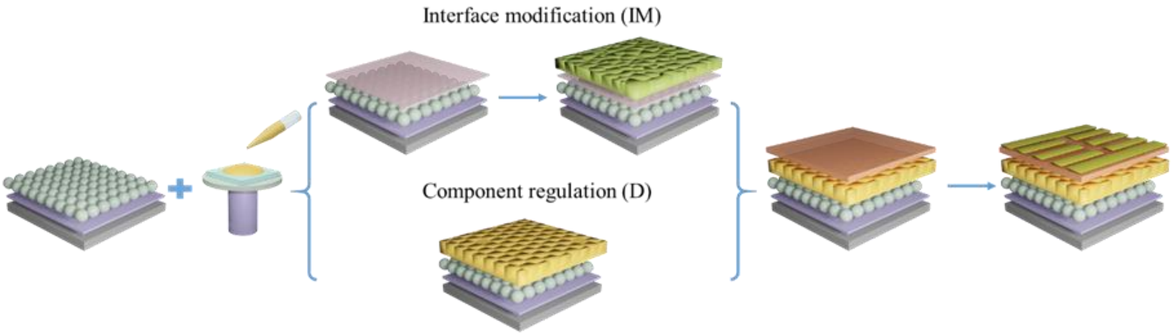

Figure 1: Schematic diagram of the perovskite solar cells fabrication.

The crystallization behavior is closely relevant to the defects density within the films and subsequent charge carrier behavior and photovoltaic performance, but few studies have focused on exploring their intrinsic connection. Herein, we introduce a pyrrolidinium-based ionic compound into perovskite component and modified the SnO_2 interface, as depicted in Figure 1, to investigate the regulation of ionic liquids in the crystal growth by using synchrotron radiation-based grazing-incidence wide-angle X-ray scattering. Through time transient measurements (TRPL, OCVD, TPV and TPC), we further probe the charge generation, transport and recombination behavior in films and devices. We find that ionic liquids manipulate the crystals growth from disordered to preferential corner-up orientation during film formation while also increasing carrier mobility, accelerating electron transport and extraction. The highest PCE achieved based on ionic liquids-containing devices is up to 21.49% accompanied by a high FF of 0.87. We observe light-induced lattice compression and crystals fragmentation in control devices via operando grazing-incidence X-ray scattering studies on both devices. While the ionic liquids-containing devices exhibited a slight light-induced crystals reconstitution and strong tolerance to light. Being exposed to the ambient conditions for up to 4368 h, the un-encapsulated $Pyr_{13}BF_4$-containing device still maintained 97% (18.04 %) of its initial efficiency. Our results reveals the crucial role of ionic liquids in crystal crystallization, carrier kinetics behavior and operational stability in detail.

Poly(propylene carbonate) solid polymer electrolyte for Lithium ion batteries

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At the present day, lithium-ion batteries are used as energy storages in a variety of scopes. They play a major role in the rapid improvement of electric vehicles and are the first choice for consumer electronics such as phones and laptops for instance. Improving the capacity and performance by either enhancing existent materials inside the battery or finding new suitable materials is an evergreen in the field of battery research.

One way to increase the performance is by replacing the common graphite anode material with Li metal although this itself is no new concept. In fact, Li metal foil was used as an electrode in rechargeable batteries in the late 1980s and, lately, is regaining more interest as an anode material because of its high specific capacity as well as its low discharge potential. [1,2] However, Li dendrite growth still remains a major safety hazard in the cells that are operated with liquid electrolyte. One mitigation strategy is to use solid polymer electrolytes (SPE) that have a higher mechanical stability in comparison to their liquid counterparts and thus, can impede Li dendrite growth. In order to achieve even higher energy densities for the Li-ion battery, Li metal anodes can to be combined with high-energy cathode materials. Albeit, the high operation potentials of those cathodes continues to be a challenge for SPE since they might cause oxidation reactions.

Poly(propylene carbonate) (PPC) has an intrinsically high oxidation voltage exceeding 4.5 V making it suitable for high voltage operation. [3] Here, SPE with PPC as polymer host and Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) as Li salt are prepared in different polymer to salt amount by drop casting method. The influence of the salt concentration on the SPE properties are studied with electrochemical impedance spectroscopy (EIS) and differential scanning calorimetry. First results have shown that the ionic conductivity increasing and the glass transition temperature is decreasing with higher amount of LiTFSI (see figure 1).

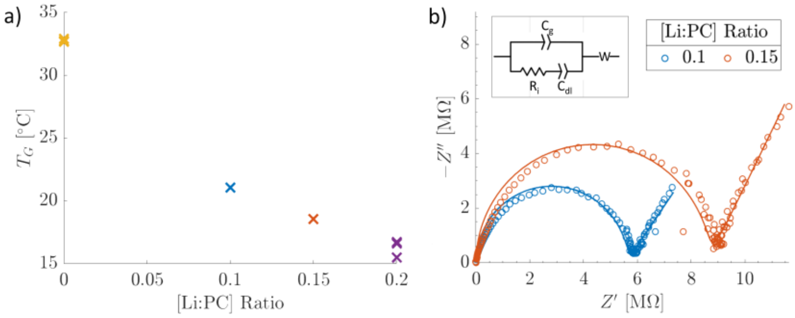

Figure 1: Glass transition temperature with increasing LiTFSI content (a) and Nyquist plot from EIS measurements (b).

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Morphology control of titanium thin films in a low temperature process

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Flexible photovoltaic devices have attracted increasing interest for their potential usage in wearable electronics, remote power, automobiles, etc[1]. Transparent plastic substrates, such as polyethylene terephthalate (PET) or polyethylene naphthalate (PEN), have been employed in various flexible solar cells. The usage of plastic substrates requires the fabrication process at low temperatures (<150℃) to avoid the deformation of substrates[2]. Moreover, a low-temperature processing route achieves the demand for devices with a reduction of energy consumption and pay-back time. However, in a conventional process, the mesoporous titania (TiO_2) films, as electron transport layers (ETLs), are fabricated with solution-processed precursors, generally followed by a high-temperature-calcination process (400-500℃) which crystalizes TiO_2[3]. To address this challenge, a low-temperature route towards mesoporous films is needed, which holds promise for simple fabrication of solar cells, such as the high-efficiency perovskite solar cells based on mesoporous TiO_2 films.

In this work, titanium thin films are synthesized at low temperature (below 100 ℃) with a polymer template sol-gel method based on the amphiphilic diblock copolymer polystyrene-b-polyethylene oxide (PS-b-PEO), in combination with selective incorporation of the titanium precursor ethylene glycol-modified titanate (EGMT). A joint process of UV treatment and water-vapor treatment is introduced to substitute the traditional high-temperature calcination. Morphology tailoring of titanium thin films in the low-temperature process is achieved by managing phase separation of the polymer template. The solvent category for the sol-gel solution is varied to tune the thin film morphologies. Scanning electron microscopy and GISAXS is used to study the structure of the titania films. The optical properties of the films are examined with ultraviolet-visible spectroscopy.

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Robust Current Control with Sliding-Mode

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Motivation

Classical proportional-, integral- and resonant controllers are widely adopted to a large range of dynamical systems. Also in power electronics applications, e.g. in Modular-Multilevel-Cascaded Converters (MMCCs) these controllers are used [1-2]. Commonly, a cascaded control consisting of an inner current control loop with PI- and PR-controllers and an outer cell capacitor voltage balancing control loop is implemented in MMCC applications. Therefore, several assumptions are made during the design procedure of the controllers, including the assumption on equality of all inductances and resistances in all phases [1-2]. However, a certain parameter uncertainty remains due to tolerances in components. Considering these tolerances during the design procedure could prevent instability but will result in a worse performance of the closed-loop system. Beside tolerances, e.g. additional grid impedance or component failures could drastically change system parameters and shift system poles towards the stability boundaries or undesired regions (e.g. oscillations).

Approach

Sliding-Mode-Controllers (SMC) could overcome these issues since these controllers are known as extremely robust against parameter uncertainties and disturbances; however, they suffer from the chattering phenomenon [3]. In order to design a robust controller with desired performance while preventing excessive chattering, a combined current controller consisting of classical P-, I- and R-controllers and a SMC is proposed for MMCCs. The structure of the approach is presented in Fig. 1. The current controller is designed in a ΣΔ- and αβγ-transformed system to decouple the DC-terminal, AC-terminal and circulating currents. An input-output linearization is applied to yield a simple integrator plant. While the DC-terminal and the AC-terminal current controllers consist of a PI-controller, the circulating current controller consists of a PI-combined with two resonant controllers (PIR) to mitigate harmonic contents. A multivariable integral SMC (ISMC) is implemented in parallel to the classical controllers that improves robustness of the system even under large parameter mismatches. This kind of SMC allows a continuous control law in parallel and prevents counteracting control actions [3]. As soon as sliding mode occurs, the closed-loop system behaves as desired and its dynamics are determined by the PI- and PIR-controllers. All uncertainties and disturbances are eliminated by the ISMC as long as the reaching condition is fulfilled.

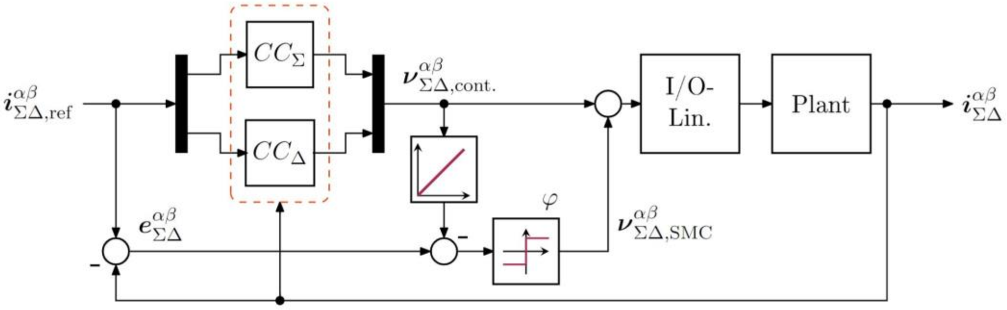

Figure 1: The proposed current controller structure

Results

Simulation results show the superior performance of the proposed approach to the classical control structure under the presence of parameter uncertainties.

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Revealing the formation kinetics of the active layer morphology for non-fullerene organic solar cells at ambient conditions

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With the advantages of highly tunable molecular energy levels and light absorption spectra, organic solar cells (OSCs) employing non-fullerene accepters have made breakthroughs of efficiencies over 18%.[1] However, the achieved best efficiency remains behind that of traditional silicon solar cells, which demonstrates the need for intensive investigation. As we know, the performance of OSCs is strongly influenced by the morphology of the active layer. Therefore, understanding the mechanism of the inner structure as well as the structure forming process of the active layer during drying kinetics is the key for device optimization. Herein, we compare chlorobenzene (CB) and chloroform (CF) used as host solvents for printing the neat films of the novel wide-bandgap donor polymer (PDTBT2T-FTBDT), the small molecule non-fullerene acceptor (BTP-4F) as well as the respective PDTBT2T-FTBDT: BTP-4F blend films. [2] Using CF, OSCs with a high power conversion efficiency of up to 13.2 % are reached in ambient conditions. In comparison to CB printed blend films, the active layer printed out of CF has a superior morphology and a more pronounced face-on orientation of the crystallites, resulting in an enhanced exciton dissociation and suppressed non-radiative charge carrier recombination.

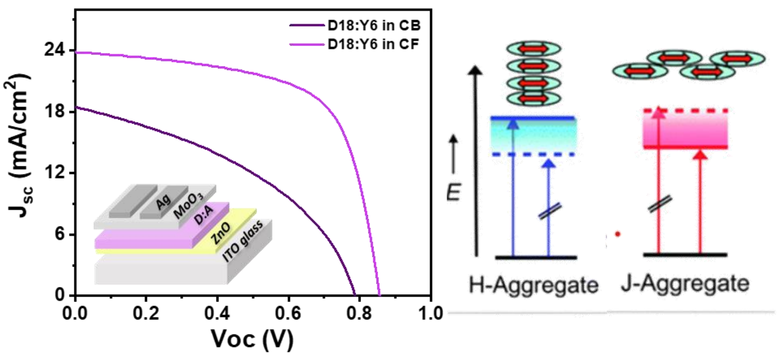

Figure 1: The J-V curves of the OSCs device based on an inverted geometry printed from CB and CF solvent, respectively.

For tracking the mechanism of the structure formation of polymer domains, we use in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and UV-vis techniques. We find that the conformational evolution of donor and acceptor is different. PDTBT2T-FTBDT preferentially forms H-aggregates and in contrast, BTP-4F prefers J-aggregates formation during solvent evaporation. Interestingly, the aggregate formation of PDTBT2T-FTBDT and BTP-4F causes a synergistic effect when printing out of CF. Therefore, the donor and acceptor in the blend thin films manifest a pronounced, well-ordered crystallite growth with a majority of the crystallites being face-on orientated. In contrast, the synergistic effect in the donor and acceptor crystallization is absent when printing out of CB, mainly because BTP-4F experiences an excessive J-aggregation. The unbalanced crystallization of donor and acceptor gives rise to a more disordered orientation with a reduced donor crystal quality. Thus, this work reveals valuable insights into the solvent effects on the donor-acceptor morphology and the mechanism of film formation kinetics in the field of non-fullerene OSCs, which cause significant differences in the related device performance.

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Construction of a thermal vacuum chamber for testing next generation solar cells under space conditions

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Next generation solar cells with better power per mass ratio are of great interest for space missions, as they can lead to significant weight and thus cost reductions. However, components needed for space missions must first be tested and verified to ensure their function under these harsh conditions. In previous experiments, not only were organic solar cells shown to be able to withstand well the UV radiation present in a unfiltered AM0 solar radiation in a laboratory environment [1], but organic and perovskite cells have also been launched on a suborbital rocket into space [2]. Following these works, in this project, a small, lab-scale thermal vacuum chamber is created, allowing the investigation of various other novel solar cell technologies in a realistic space environment simulation. In addition, a way to relate previous space experiments to laboratory experiments will be given with the newly established set-up.

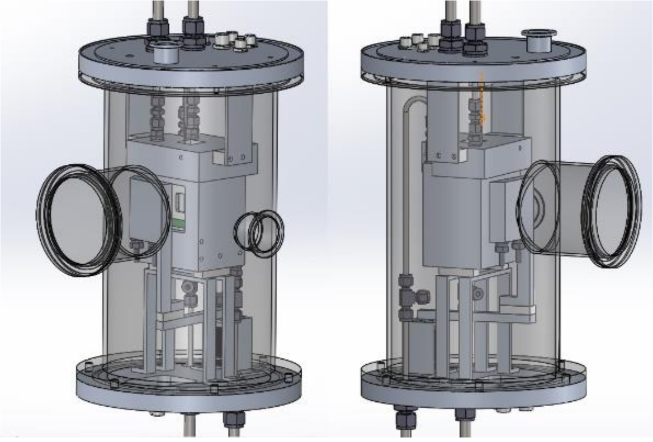

Figure 1: CAD model of the chamber

The test environment is defined by a high vacuum at pressures of less than $1x10^{-5}$ hPa, while the cold background of space is simulated by a liquid nitrogen (LN2) cooled thermal vessel with a highly absorbing surface coating. To imitate thermal radiation from Earth for low Earth orbit simulations, an electrically heated thermal plate can also be additionally inserted. Heating from solar radiation can either be simulated by means of an AM0 Sun simulator or by electrically heating the entire thermal vessel to the desired temperature. To recreate the high thermal stresses, most satellites are subjected to continuous cycling between the direct illumination from the Sun and cold environment in Earth's shadow. The LN2 and electric heaters of the thermal vessel can be used to run a thermal cycling program. This way, long-term simulations with thermal cycles can be run.

This system allows us to reliably test novel solar cells under realistic, space-like condition. The performance of the solar cells can be measured under varying external environmental influences, allowing us to recreate the degradation behavior the solar cells would experience during a spaceflight. The test environment for in-operando measuring the behavior of the solar cells is fully modular, allowing the thermal vacuum chamber to be easily adapted to other cell geometries.

Also, by injecting different gases into the thermal vacuum chamber, a controlled atmosphere to simulate alternative environments can be achieved. Thus, by changing the intensity from solar illumination, different environmental conditions as for example on the Martian surface can be recreated, allowing a wide range of possible applications the solar cells can be tested for.

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Antisite Li/Ni disorder in delithiated $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (0<x<1) battery cathodes

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Facing the emission of greenhouse gases that cause global warming and climate change, the replacement of internal combustion engines with electric motors is of particular interest on the road to a green future. Therefore, energy storage devices like lithium-ion batteries experience an increasing demand on higher energy and power densities as well as lower costs, which resulted in the development of the state-of-the art lithium-ion batteries with $Li_xNi_{0.8}Co_{0.15}Al_{0.05}O_2$ (NCA) and graphite electrode chemistry that are used for instance in electric vehicles like the Tesla Model S [1, 2]. Nevertheless, the electrochemical efficiency of Li-ion batteries is largely determined by the diffusivity of Li-ions and the transport of electrons between the electrode materials inside the cell. In nickel-containing cathode materials mixed Li\Ni occupations are often occurring, which leads to structural disorder, the blocking of the 2D diffusion pathways of Li^+ by Ni^{2+}, as well as the reduction of the cell capacity and the structure stability. Mixed transition metal batteries like high nickel content Li(Ni, Co, Al)O_2 and Li(Ni, Mn, Co)O_2 are considered to be promising cathode materials showing better cycling stabilities, lower toxicity, lower costs etc. and are therefore of particular interest from the viewpoint of Li\Ni disorder [3, 4]. In literature, the studies and understanding of factors causing cation mixing, especially for high nickel content lithium ion batteries, is still controversial and poorly presented. In the current contribution, extracted NCA cathode material from 18650-type Li-ion cells was analyzed by a systematic *ex-situ* neutron powder diffraction study with the high-resolution neutron powder diffractometer SPODI at FRM II research neutron facility. The structural data will be presented and discussed together with their electrochemical characteristics. Structural parameters were collected by using the full-profile Rietveld refinement method. While the refined lithium concentrations, representing the electrochemical state of the cell, were found to decrease linearly and to agree well with the chemical reference obtained by an ICP-OES method (Fig. 1), there is no major change in concentration of the refined transition metals visible during the electrochemical cycle.

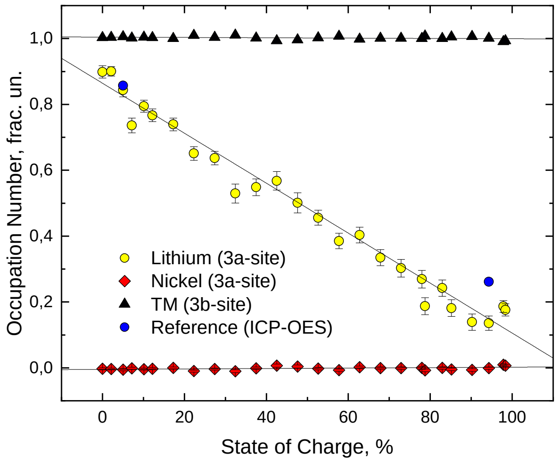

Figure 1: Lithium and transition metal occupations as a function of state-of-charge with two ICP-OES chemical references

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Design of an electric submersible pump motor for geothermal energy plants

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As part of the German energy transition, fluctuating energy sources such as photovoltaics and wind energy are increasingly being used. This raises the question of how the base load can be reliably covered in the future. Due to the permanently available geothermal energy, deep geothermal energy represents a possibility to provide part of the base load. For this to be successful, it is crucial that geothermal power plants are highly reliable and require little maintenance.

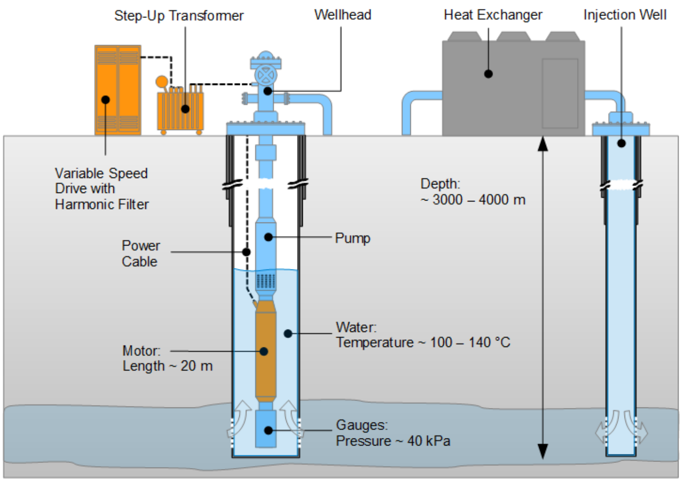

Figure 1: Schematic of a geothermal power plant

However, there are regular failures of these power plants. The reason is that the service life of pump systems currently in use is two years or even less. One cause is the electric motor that drives the pump unit. The motor is mounted at the end of the production well at a depth of several thousand meters and fails due to the extreme environmental conditions. In such a case, the entire motor has to be transported to the surface and replaced, which can result in an outage lasting several days [1]. To improve the reliability of geothermal plants, a new electric motor is therefore being designed which, in addition to being more efficient, should also have a higher thermal load capacity.

The motor is designed using a multiobjective genetic algorithm with the help of FEM simulations. At the beginning the motor is optimized with regard to the most important target parameters machine torque m_m and power factor $\cos(\Phi)$. While various basic parameters, such as the number of slots, are kept constant, other parameters, such as the slot shape or the number of windings, are varied. After a first run of the genetic algorithm, the design space is narrowed down further and a new optimization loop is performed. The results are then presented as a pareto front. A comparison of the results fulfilling the requirements shows that there are different design variants that achieve or also exceed the required main target variables. In order to finally select a suitable design variant, a further consideration of additional targets within the solution space is necessary. For this, factors such as torque ripple, efficiency and thermal load capacity must be considered in the future.

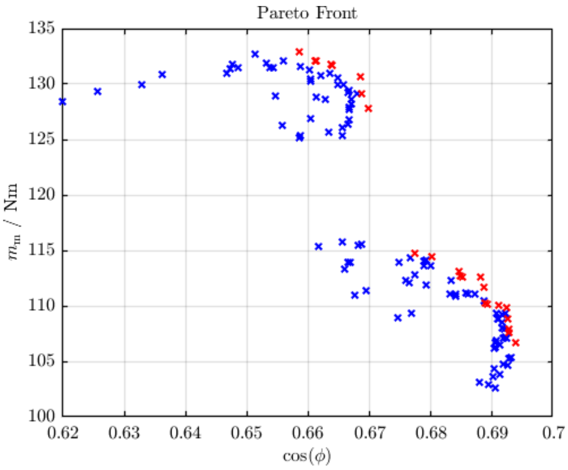

Figure 2: Pareto front as result of design optimization

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Polymeric zwitterions as electron transport layer in PBDBTCl-DTBT:BTP-4F organic solar cells

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Until now, polyzwitterions (e.g. polysulfobetaines) have been mostly used in biological and medical applications as anti-fouling agents [1]. Their anti-fouling properties originate from their strong hydrophilicity. In addition, they are electronically neutral although they carry permanent positive and negative charges. The presence of permanent charges induces a strong dipole moment on the macromolecular backbone, as every monomer of the polymer carries a side chain with a permanent positive and negative charge [2].

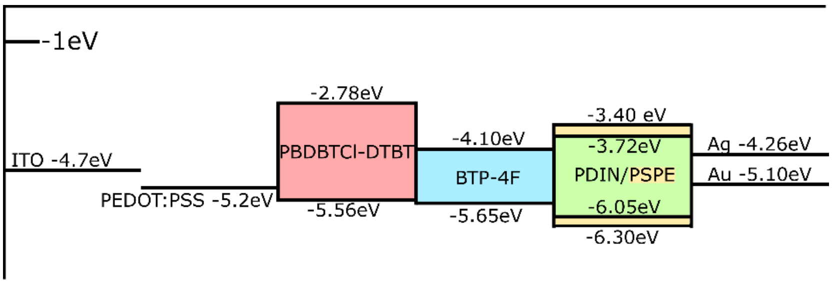

Figure 1: Energy diagram of the solar cell components[3]

In this work, we study the optoelectronic properties and morphology of one specific polysulfobetaine (PSPE), in solutions and films, to be later on used in an organic solar cell device. Here the permanent dipole moment of PSPE might be able to facilitate electron transport from the active layer to the electrode, thus working as an electron transport layer (ETL). This will be investigated in a organic solar cell using a PBDBTCl-DTBT:BTP-4F active layer. The architecture of the solar cell is supposed to be ITO/PEDOT:PSS/Active Layer/PSPE or PDIN/Ag. The energy bands of this setup can be seen in Figure 1. This architecture is known to be able to reach peak power conversion efficiencies (PCE) of PCE = 17.12% with PDIN [3].

To fully explore the morphology and optoelectronics of the different layers various characterization techniques are utilized. Figure 2 shows a Tauc plot recorded from UV-vis data for a drop-cast PSPE film. Here a representation for an indirect bandgap was used. From the intersection between the fit and the Energy axis, an indirect band gap energy of $E_g = 2.90$ eV can be determined. This is comparable to the band gap energy of PDIN. Further spectroscopic investigations include UV and X-ray photoelectron spectroscopy, impedance spectroscopy and photoluminescence.
The morphology is assessed by X-ray reflectometry, grazing incidence small/wide angle X-ray scattering, optical and atomic force microscopy.

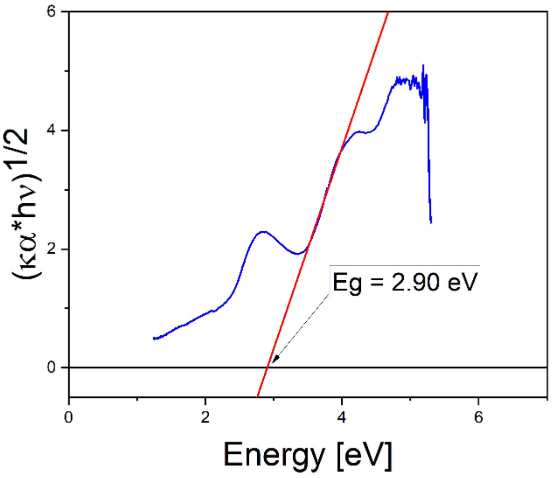

Figure 2: Tauc-plot of the indirect bandgap in dropcasted PSPE film

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Improving morphology and efficiency of slot-die coated Perovskite Solar Cells

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In industry and research of sustainable power production, perovskite solar cells (PSCs) got a lot of attention in the last couple of years, due to their low material cost, low weight, high power conversion efficiencies (PCEs), and high specific power. Additionally, simple solution-based deposition techniques like slot-die coating or spray coating can be used to produce solar cells [1]. Using minimal material, being fast and having the possibility of up-scaling makes slot-die coating one of the most promising fabrication technique, achieving PCEs up to 21% [2] and therefore reaching PCEs of silicon based solar cells.

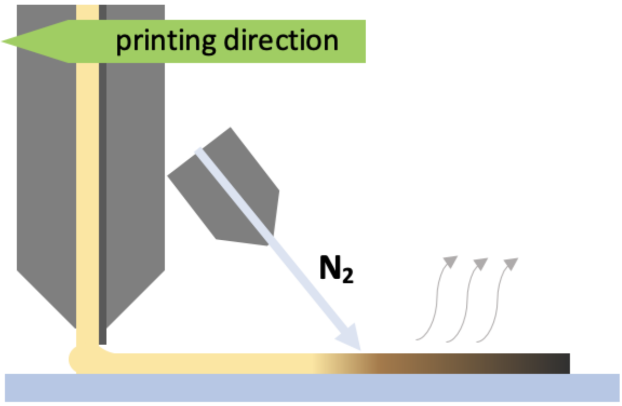

Figure 1: Schematic of slot-die coating process.

In this work, we compare slot-die coated PSCs with different perovskite compositions. In particular, the solutions of the perovskite layer contain different ratios of lead iodide (PbI_2), methylammonium iodide (MAI), formamidinium iodide (FAI), and methylammonium chloride (MACl) in a solvent mixture of 2-Methoxyethanol (2-ME) and dimethyl sulfoxide (DMSO). To improve the film quality of the printed perovskite layer, the influence of nitrogen gas quenching is extensively studied and the process optimized. The resulting high-quality thin films are analyzed with optical and structural characterization methods like spectroscopic and X-ray scattering methods. To gain complementary information about the PSCs, current-voltage and external Quantum Efficiency measurements are carried out.

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Organic Solar Cells on Flexible Substrates

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Latest progresses in the development of organic solar cells (OSCs) have led to power conversion efficiencies (PCEs) of over 18% with an upward trend. [1] The material and corresponding energetic structure of a typical OSC can be seen in figure 1. In combination with the ease and low cost of production, the possibility of flexibility and the light weight of OSCs, they turn into a serious alternative to silicon solar cells. One approach to further improve the light weight feature is to replace rigid substrates with flexible ones like PET or PEN. This could widen the range of portable and aerospace application possibilities of OSCs.

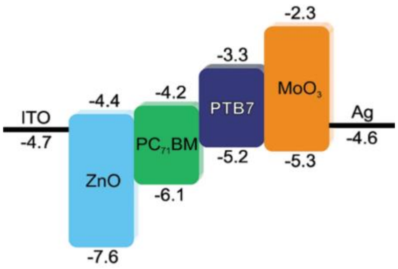

Figure 1: Material and energetic structure of a typical OSC [2]

Due to low toxicity, easy preparation, high carrier mobility and high chemical stability ZnO has shown to be one of the best choices for the electron transport layer (ETL) in inverted OSCs. The conventional way to prepare the ZnO film on a heat resistant substrate is the sol-gel method. A ZnO precursor solution is applied onto the substrate and then annealed at up to 200°C for 1 hour. [2] Since PET and PEN have glass transition temperatures of 69°C and 113°C respectively and and are long term heat resistant at a maximum of 120°C and 155°C respectively [3] a possibility to produce a nice ZnO film at low temperatures is desirable.

One alternative way to produce ZnO thin films at low temperatures is to synthesize ZnO nanoparticles and spin-coat a solution of those onto the substrate. The ZnO film then can form without annealing. It was shown on rigid substrates the OSCs with ZnO ETLs produced by using ZnO nanoparticles provide even higher PCEs than the ones with ETLs prepared by the sol-gel method (see Figure 2). The higher PCEs can be attributed to the originally higher crystallinity and therefore higher carrier mobility in the nanoparticles which leads to a lower recombination rate. [2]

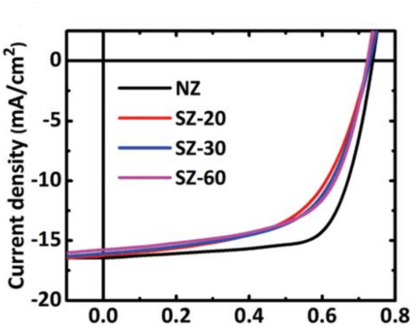

Figure 2: Current-Voltage-Characteristics of the OSCs prepared with the nanoparticle method and the sol-gel method with different annealing times [2]

Using synthesized ZnO nanoparticles allows us to grow ZnO ETLs at low temperatures that have higher crystallinity than than the ZnO films prepared using the sol-gel method. Due to higher mobility and therefore lower recombination rate this technique provides the possibility to realize OSCs on light weight flexible substrates that have the same or even higher efficiencies than the OSCs on rigid substrates built using conventional methods.

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Printing of perovskite layers for solar cell application

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Perovskite materials are new as light absorber materials in solar cells. This material class with the chemical composition ABX_3 has been first introduced in solar cells a decade ago and has met with tremendous success. Perovskite solar cells (PSCs) can reach power conversion efficiencies of over 25%. Electrons are strongly absorbed (high absorption coefficient, direct bandgap) by this material class and move relatively easily through the material (high charge carrier mobility and large diffusion length). Additionally, many semiconductor properties are tunable by elemental substitution of the ABX_3 composition. With these advantages, research is pushing towards market-ready solar cells. Until now, modules with a larger active area above 15% can be manufactured. However, new deposition techniques need to be developed to achieve the goal of fast, flexible, and resource-efficient solar cell fabrication.

Slot-die coating is one promising thin-film deposition technique in which the solution-based ink is pushed through a thin slit onto a moving substrate. The material then crystallizes from the drying ink, and a thin film forms. Perovskite materials can be deposited in a multi-step process from lead iodide (PbI_2) and methylammonium iodide (MAI), shown in Fig. 1a. We investigate the crystallized thin films with X-ray scattering methods on a 2D detector, which helps us identify the crystalline materials present in the film, (Figures 1b and 1c).[1-2] In Figure 1c, we can see the disintegration of the DMSO-containing precursor phase and the formation of the perovskite phase (red). Single cuts, as depicted in Figure 1c, can be plotted over time to show the perovskite material formation (Figure 1d). We developed a python-based software tool for processing 2D grazing-incidence wide-angle X-ray scattering data, which is called INSIGHT.[3] The features implemented in INSIGHT aim at complete coverage of scientific needs from the experiment to publication-ready plotting of extracted data. A common workflow involves visualization of raw data and transformation to q-space (reshaping) for the extraction of crystallographic-relevant information.

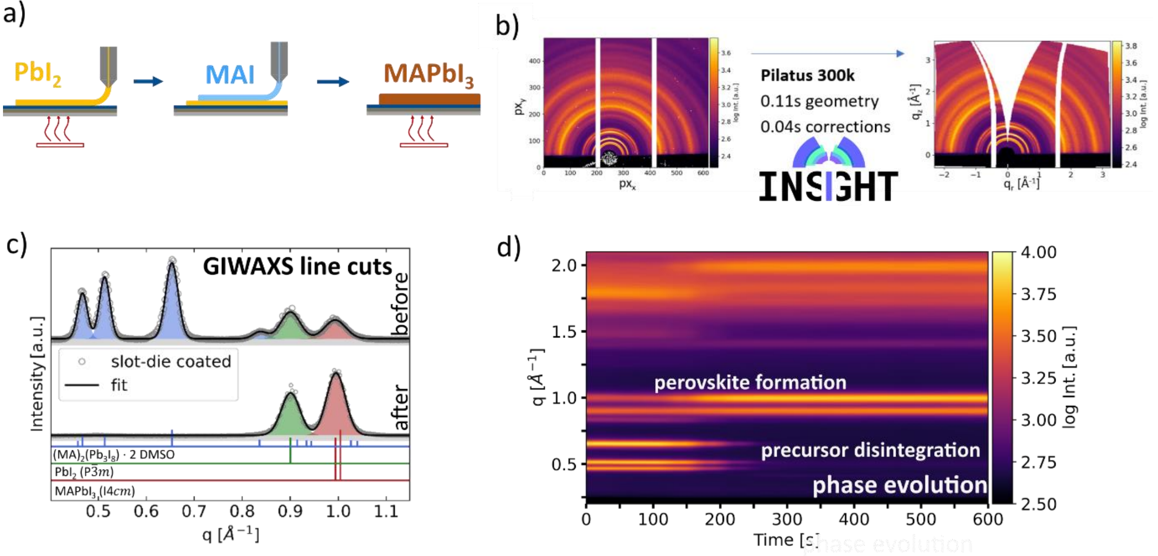

Figure 1: a) Multi-step slot-die coating of perovskite absorber layers for solar cell fabrication. b) Transformation of 2D X-ray scattering data to reciprocal space. c) Cuts of 2D data before and after the annealing step. Perovskite (red) forms while the precursor (blue) disintegrates.[3] d) Time evolution of cuts which shows the disintegration of the precursor and the formation of perovskite material.

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Analyzing the simplification of context shading for use in building energy simulation

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Energy simulation methods can demand high computing capacities and be time-consuming. Oversimplification of integrating the context shading, like surrounding buildings and trees, can lead to inaccurate estimations in the energy demand of buildings. On the opposite, a detailed representation of shading objects demands additional information with extensive simulation periods. Methods focusing on reducing simulation times require simplified in- and outputs for shading, e.g., the recently developed voxel methodology [1] or machine learning approaches [2]. Therefore, we want to clarify whether shading from surroundings can be represented in a single transparency value for each façade direction. To address this issue, a parametric study of the influences of different shading scenarios was performed.

Figure 1 shows the evaluated scenarios. Following the hypothesis that the effect of shading on a façade is comparable to the impact of a façade´s transparency, five base cases for different window-to-wall ratios (WWR) were analyzed. By changing the degree of transparency or shading, 20 iterations for each case were simulated.

The results show the degree of correlation between the models. It deviates with increasing WWR, as shown in Figure 2. Thus, we conclude that the hypothesis of representing context shading by single transparency values is more accurate for small WWRs. Further research should focus on the non-linear behavior to conclude on the proposed simplifications validity.

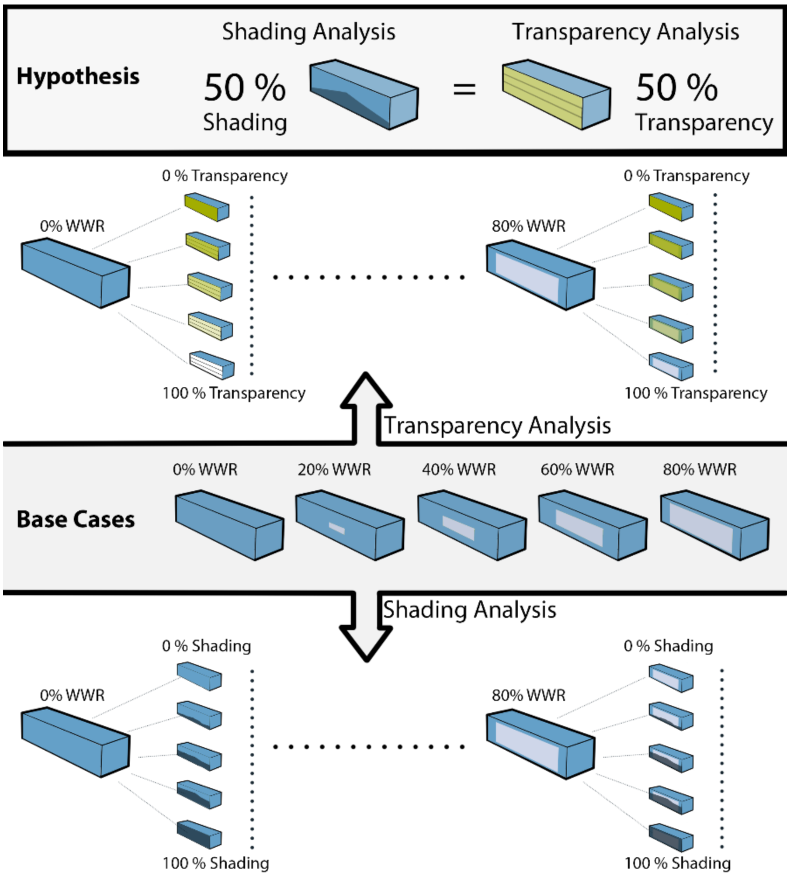

Figure 1: Analysis of different shading approaches

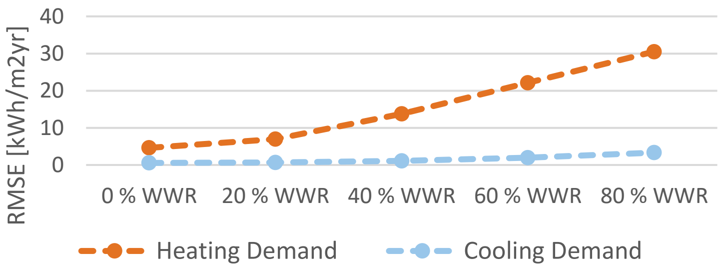

Figure 2: Root Mean Squared Error (RMSE) of building energy simulations with varying Window to Wall Ratios (WWR)

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Hybrid thin films for H_2 evolution applications

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Photocatalysis of water is becoming one of the leader fields in term of green approaches to obtain sustainable energy. The water splitting reaction is an easy way implement the sun to produce hydrogen-based energy. Numerous photocatalyst has been reported for this purpose. Recently, Pt loaded graphitic carbon nitride (g-CN) has been found has a promising candidate for H2 evolution under visible light.[1] The latter showed a great H_2 evolution efficiency in aqueous solution despite the photocatalyst spreading issue in solution. Previous works proposed to introduce hydrogels as host matrix and water supply for water splitting reaction with g-CN.[2,3]

The aim of this work is to bring this material in a polymer thin film configuration in order to make it suitable for industrial purposes. Poly(N-isopropylacrylamide) (PNIPAM) already exhibits good swelling capacity in water vapor exposure and seems to be a suitable polymer for such a hybrid thin film system.[4] A new isomer of the latter, poly(N-vinylisobutyramide) (PNVIBAM) raised our attention due to its higher lower critical solution temperature (LCST) in aqueous solution (≈ 39°C) which makes it more stable in ambient environment. Therefore, PNVIBAM could also be the host matrix for g-CN photocatalyst. Spray coating has been chosen to be the film deposition technique of hybrid films such as PNVIBAM/g-CN/Pt and PNIPAM/g-CN/Pt. A comparative study of those two hybrid films is presented in term of spray coating parameters, photocatalyst and polymer concentrations. Grazing incident small angle x-ray scattering (GISAXS) is the main tool of this investigation. G-CN/Pt blended polymer films structure is analysed in static measurement as well as under light irradiation condition.

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In-situ investigation of degradation in active layers for organic photovoltaics, produced with binary solvent additive

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In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active materials due to their superior performance compared to e.g. planar layered devices. In this optically active polymer layer, a photon is absorbed and an exciton created. After diffusion to a donor-acceptor interface, the exciton is dissipated and charge carriers can be extracted at the electrodes. A promising low-band gap electron donor material is PTB7 ($(C_{41}H_{53}FO_4S_4)_n$). We investigate films of PTB7, blended with PCBM, an electron acceptor fullerene molecule, prepared out of chlorobenzene solutions with and without 1,8-diiodooctane (DIO) and diphenyl ether (DPE) as binary solvent additive. The addition of solvent additives has been proven to improve the blend microstructure, which leads to higher power conversion efficiencies of the respective photovoltaic devices. On the other hand, DIO and DPE have higher boiling temperatures than the bulk solvent, thus tend to remain in the film during the drying process[1,2]. The effect of residual solvent additives on structure, dynamic and performance evolution has been discussed before. [3,4] We investigated the influence of the drying procedure on the chemical and physical degradation during illumination in ambient conditions. UV-vis, Raman and FTIR spectroscopy was used to identify optical properties and the chemical bond structure.

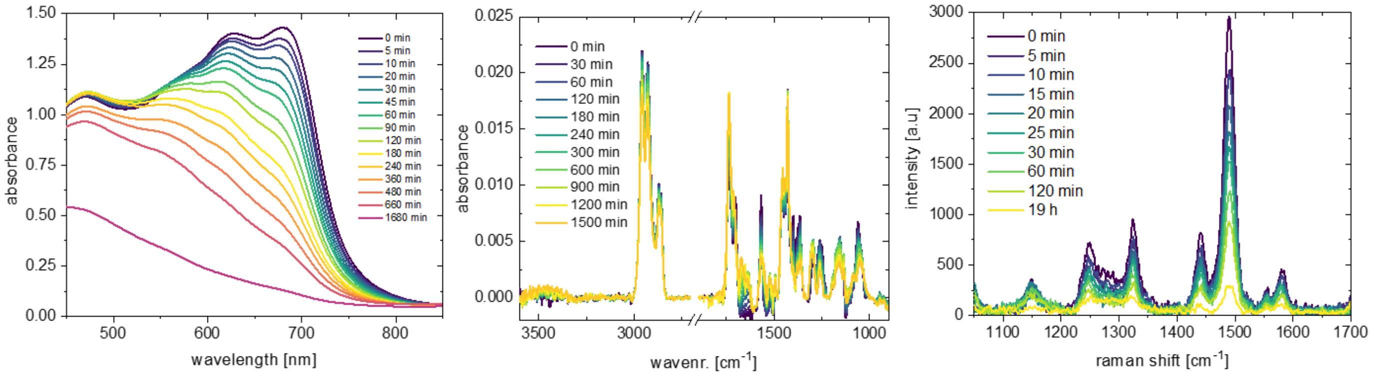

Figure1: *Optical (a) and infrared (b) absorbance spectra and Raman scattering intensity of a PTB7:PCBM blend film, produced with binary solvent additive DIO:DPE. Films were illuminated for the indicated time by a LED light source or by the Raman laser, respectively, and probed in-situ.*

Examples for the evolution of the respective properties of a well dried PTB7:PCBM blend film, produced with binary solvent additive, are given in Figure1. Figure 1a) shows the evolution of the optical absorbance in the visible spectrum, whereas Figures 1b) and 1c) display the evolution of the IR-absorption and Raman spectra. It is clearly visible, that all samples degrade over time upon illumination with a LED light source (UV-vis & FTIR) or the Raman laser (Raman). It is evident, that the properties of the active layer change during illumination. This development is tracked for various drying procedures and the possible influence of residual solvent (-additive) is discussed.

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Fabrication of Plasmonic Nanostructures in Perovskite Solar Cells

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Plasmonic metal-dielectric composites have fascinated a great interest in photovaltics, owning to surface plasmon resonance (SPR) induced by incident radiation. [1] The plasmon induced electric excite could be changing photoenergy localization and the lifetime of excited states materials. In recent years, the state-of-the-art power conversion efficiencies (PCEs) of photovoltaics, such as organic solar cells (OSCs) and perovskite solar cells (PSCs), have been rapidly enhanced by interfacial engineering, optimizing device processing and developing new active layer materials.[2] Light management in perovskite solar cells (PSCs) is an essential issue for achieving higher efficiency and the utilization of plasmonic metal nanostructures is a promising approach for enhancing light harvesting. Thus, the development of facile and scalable fabrication methods that enable integrate the highly-dispersed plasmonic metal NPs into PSCs is highly desirable but yet remains challenging.

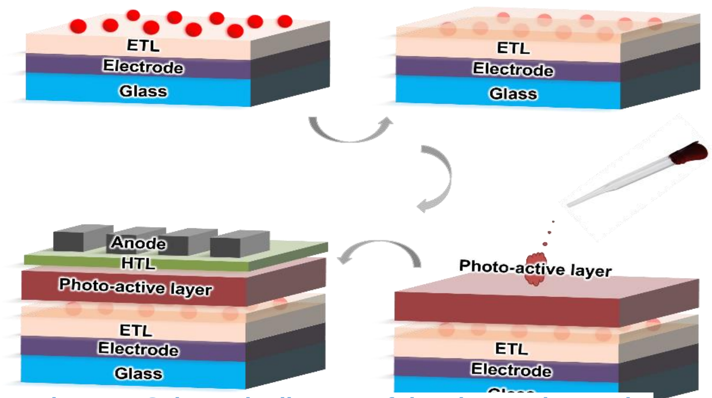

Figure 1: Schematic diagram of the plasmonic metal nanoparticles enhanced photovoltaics.

In view of this point, to regulate the plasmonic spectra of Au NPs for maximizing the enhancement in light-absorption of active layer, we assembly the metal NPs onto the electron collecting layer to broaden absorption band of photoactive layer of PSCs as well as enhance the device performance as is shown in Figure 1. To meet the optimal results, we put effort into the plasmonic structure regulation, since the size, density, and morphology of the Au NPs will influence the crystallinity of the photoactive film and charge transportation of the device. In order to investigate the possible influence of the sizes of Au NPs on subsequent films and device performances, as is shown in Figure 2, we can see that the well-dispersed Au NPs with different sizes were visibly assembled on the silica surface. In addition, grazing incidence wide angle x-ray scattering (GIWAXS) is used to probe the crystalline structure of the perovskite active layers. Grazing incidence small angle x-ray and neutron scattering (GISAXS) is used to study the quality of the interface in terms of contact area between the materials.

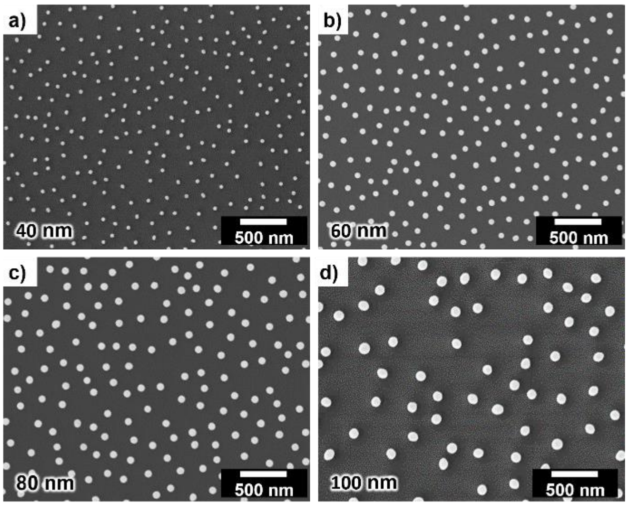

Figure 2: SEM images of Au NPs assembled on the sunstrates with different sizes a) 40 nm b) 60 nm c) 80 nm d) 100 nm.

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Graphitic Carbon Nitride (g-C_3N_4): Thin-Film Fabrication

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A polymeric semiconducting material called graphitic carbon nitride (g-C_3N_4) has drawn enormous attention of the researchers who are endeavouring for a clean and inexhaustible energy resource. The unique property of this material is being environmentally benign due to its metal-free nature, and high solubility in water, a green-solvent [1]. Moreover, the earth-abundance of carbon and nitrogen enables easy and environmentally friendly synthesis at low costs.

The astonishing electronical, optical, and physiochemical properties as well as high thermal, physical-chemical stability render g-C_3N_4 as a prime center for the extensive applications of photocatalytic water-splitting, oxygen reduction, and biomedical and sensing research [2]. With absorption in UV-visible region g-C_3N_4 exhibits a band-gap energy of 2.7eV, this material with promising properties can also be utilized as a photovoltaic performance booster for solar cells applications [3].

Fabrication of homogeneous g-C_3N_4 thin-films with tailored thickness and morphology is important to develop novel applications for future clean energy technologies. However, the material deposition to achieve homogeneous thin films is challenging, rendering information about the bulk material properties essential for device application largely unknown. In this work, the promising slot-die coating method will be employed to get homogeneous and pin-hole free films with good adhesion onto the substrates. Slot-die coating is a low-waste high-throughput manufacturing technique that allows fine-tuning film properties. The deposition method and final thin-film properties are compared to classical lab-scale spin-coating in terms of spectroscopic and morphological characterization methods.

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Printed mesoporous hybrid films obtained via sol-gel route for photovoltaic application

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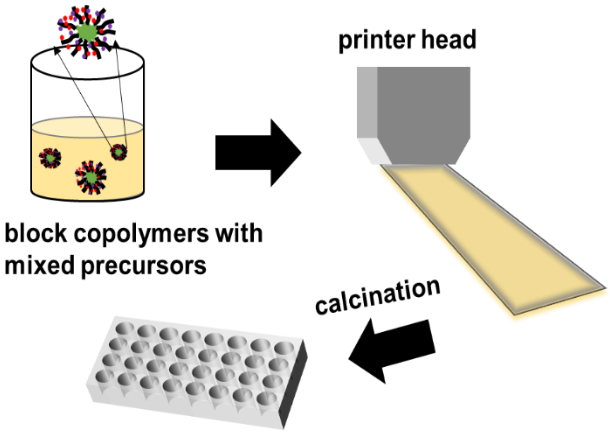

Figure 1: Schematic illustration of the fabrication process for the zinc/titanate films with tunable mesoporous via sol-gel synthesis.

Mesoporous films containing titania dioxide or zinc oxide are successfully synthesized via sol-gel technology.[1] Researchers are interested in using these films in the photovoltaic area since titanium dioxide and zinc oxide have a high potential for applications in photocatalysis, solar cells, sensors, etc., due to their semiconductive properties.[2] We investigated the morphologies of the mesoporous hybrid films obtained by calcining the hybrid films printed from a solution containing poly(styrene)-b-poly(ethyleneoxide) PS-b-PEO and two types of precursors with different ratios, zinc acetate dihydrate and titanium isopropoxide.[5] The amphiphilic diblock copolymer PS-*b*-PEO self-assembles in core-shell micelles in a selective solvent, and the precursors is loaded in the micelles due to hydrogen bonds.[3, 4] The details of the core-shell micelles copolymers with and without precursors in solution were probed using small-angle X-ray scattering.

We also investigated the morphologies of hybrid films fabricated using slot-die printing and the mesoporous hybrid films after calcination using grazing incidence small-angle X-ray scattering and scanning electronic microscopy. The film thickness, crystal phase, chemical composition, and optical properties were characterized using X-ray reflectivity, X-ray diffraction, Fourier transform infrared spectroscopy, and ultraviolet-visible spectroscopy, respectively.

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PHIL implementation of a decentralized online OPF for active distribution grids

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This paper demonstrates a Power Hardware-in-the-Loop (PHIL) implementation of a decentralized optimal power flow (D-OPF) algorithm embedded into the operations of two microgrids connected by a tie line. While D-OPF has been extensively studied [1], to the best knowledge of the authors, a Power Hardware-in-the-Loop(PHIL) implementation in a realistic grid setting has not yet been attempted. Porting the online D-OPF algorithm into a real-time (RT) PHIL application requires further considerations, generally neglected in the simulation models. Another challenge is the integration of the static optimization problem running in a PC into a RT control scheme for PHIL testbeds which run on embedded RT targets.

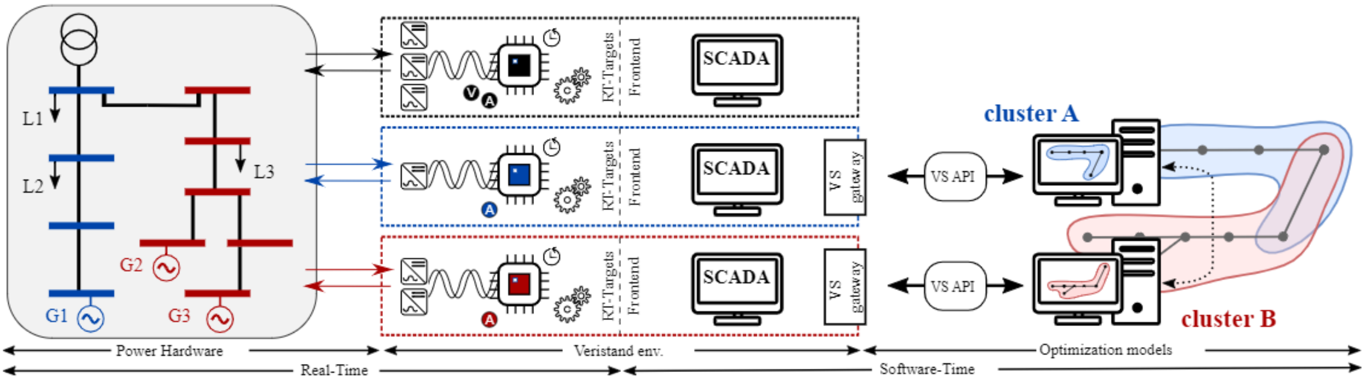

Figure 1: PHIL implementation of online D-OPF in CoSES: Microgrid clusters with PHIL generator and loads (left), real-time control setup (center), ADMM based D-OPF optimization (right)

To integrate the static behavior of the optimization model, a two layer control architecture is introduced. Underneath the dispatch commands from the D-OPF, a primary control scheme provides instantaneous reaction to the load dynamics. This setup is tested in the PHIL environment of the CoSES Lab in TU Munich [2]. In the experiment, the two microgrids cooperatively optimize their operation through an Alternating Direction Method of Multipliers (ADMM) based unbalanced D-OPF [3]. The operation is then benchmarked against the exclusive use of primary control, without D-OPF. The decentralized approach outperforms, reducing generation costs by 6%, but also shows minor inefficiencies of integrating optimization methods into the real-time operation of the system.

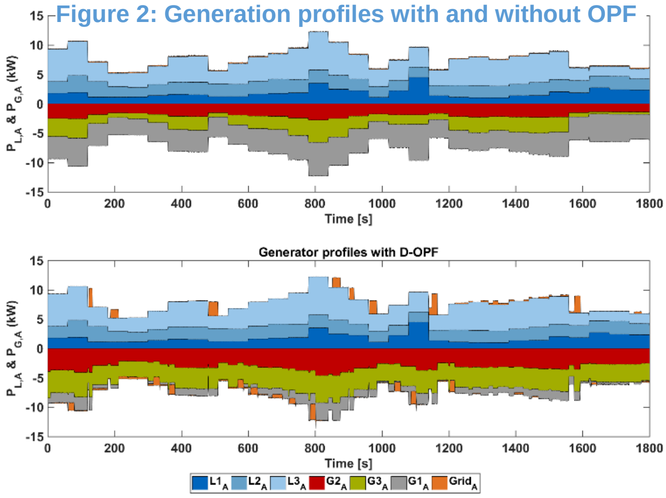
Figure 2: Generation profiles with and without OPF

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Low-Temperature and Water-Based Biotemplating of Nanostructured Foam-Like Titania Films using ß-Lactoglobulin

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Titania nanostructures are broadly used in energy-related applications, such as anodes in solar cells and batteries, in hybrid thermoelectric devices, or in the photocatalytic production of hydrogen. A tailored titania morphology that matches required charge diffusion lengths and degree of crystallinity are beneficial for efficient performance. Especially foam-like films show beneficial morphology because of their high surface-to-volume ratio, resulting in a large interfacial area between subsequent layers inside the working device's stack. Nanostructured foam-like titania films can be achieved, e.g., by established diblock copolymer-directed sol-gel synthesis. However, this synthesis route usually involves harmful organic solvents and sintering at high temperatures.

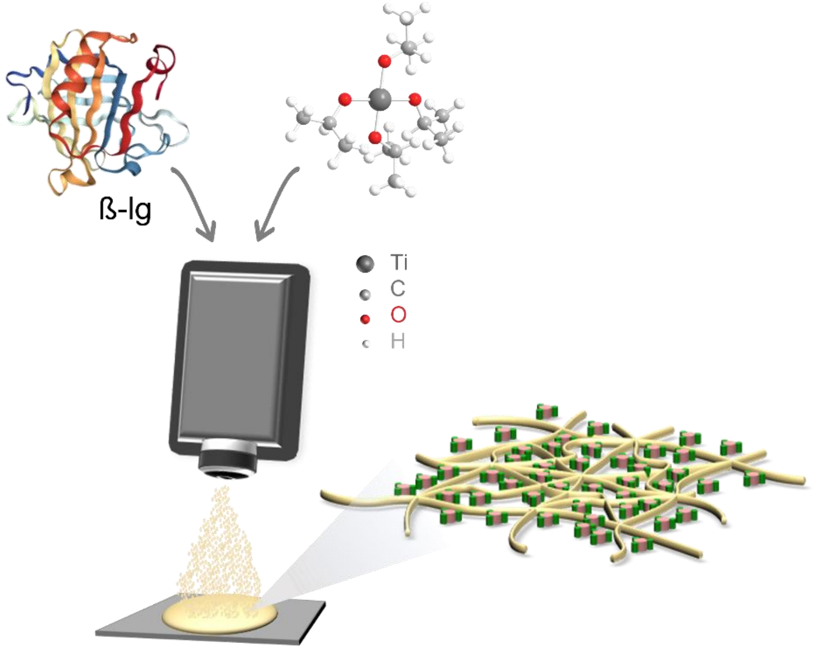

Figure 1: Bovine whey protein ß-lactoglobulin is introduced as biotemplate in the water-based synthesis of crystalline and foam-like titania structures during spray deposition.

We use a low-temperature and water-based synthesis route based on biopolymer templating and spray deposition to promote an environmentally friendly and sustainable approach to nanostructured and crystalline foam-like titania films. [1] An established titania precursor is mixed in acidic water with the water-soluble bovine whey protein ß-lactoglobulin (ß-lg), used in the food industry as a texture and foaming agent. The water-solubility of ß-lg matches the aqueous media needed for the titania precursor to precipitate in crystalline titania at low temperatures. The biopolymer matrix built up of ß-lg sterically directs the titania morphology during spray deposition and is removed afterward by UV-light exposure. With this, nanostructured and crystalline titania films with foam-like morphologies are achieved at low temperatures. Spray deposition enables a sustainable deposition of low wastage suitable for fabricating foam-like titania on an industrial scale.

We perform simultaneously *in situ* grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS) to understand film formation kinetics during the spray deposition on the nano and crystalline length scale. The results complement scanning electron microscopy (SEM) and explain the templating role of ß-lg and the growth of titania crystallites inside the biohybrid film.

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Grazing incidence x-ray scattering on lithium iron phosphate electrodes

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Lithium-ion batteries turned out as an indispensable energy supplier in modern society which however suffers from safety concerns due to the flammability of the liquid electrolyte. Solid polymer electrolytes (SPEs) can bypass this obstacle and therefore represent a serious alternative to conventional electrolytes. Especially single-ion conducting polymers (SICPs), which have the anion covalently bonded to the backbone of the polymer and thus exhibit a theoretical transference number of unity, attracted strong interest in battery research. However, a major drawback of polymer-based batteries is the poor interfacial contact between electrode and polymer electrolyte. Therefore, the polymer electrolyte is often used as binder in the slurry preparation instead of the neutral and non-conducting polyvinylidenfluorid (PVDF) in order to enhance ion conduction in the electrode and decrease the interfacial contact resistances. It is known, that a 1:1 wt% mixture of PVDF and a single-ion conducting polymer results in superior battery performance.[1] In this study, lithium iron phosphate (LFP) cathodes with different weight ratios of PVDF and the SICP poly((trifluoromethane)sulfonimide lithium styrene) (PSTFSILi), as binders are prepared and analysed with real (scanning electron microscopy) and reciprocal (grazing-Incidence small/wide angle X-ray scattering) space techniques. Specifically, a series of six LFP electrodes with LFP: carbon black: polymer = 80:10:10 and different weight ratios of PVDF and PSTFSILi is manufactured and GISAXS/GIWAXS is performed. By modelling the horizontal line cuts at the Yoneda peak position of LFP at $q_z = 0.45\ \mathrm{nm}^{-1}$, morphological information dependent on the polymer ratio can be obtained. These results can help for a better understanding of electrochemical impedance spectroscopy (EIS) data.[2]

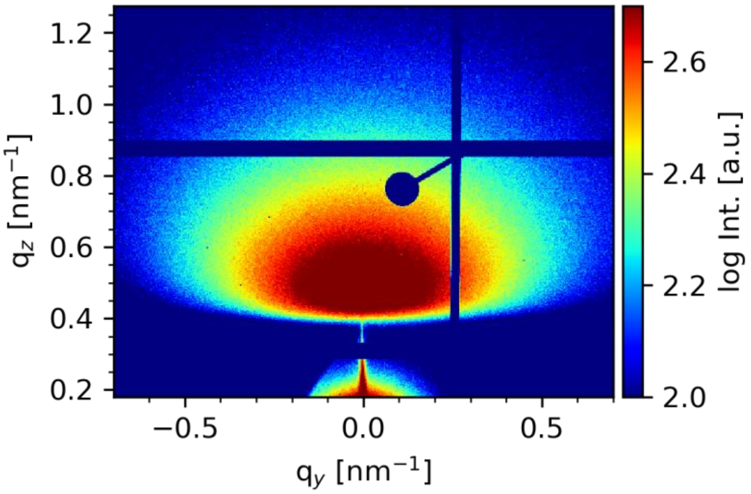

Figure 1: GISAXS detector image of a LFP electrode. The absence of a specular peak indicates a high surface roughness.

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Improvement of the thermoelectric properties of PEDOT:PSS films via DMSO addition and DMSO/salt post-treatment resolved from a fundamental view

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Organic semiconductors have attracted intense attention due to their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, poly(3,4-ethylene dioxythiophene):poly(styrenesulfonate)(PEDOT:PSS) is the most studied conducting polymer system due to their intrinsically high electrical conductivity, low thermal conductivity, and high mechanical flexibility[1,2]. The combination of DMSO-solvent doping and physical-chemical DMSO/salt de-doping in a sequence has been used to improve the thermoelectric PEDOT:PSS films. A high power factor of ca.105.2 µW m^{-1} K^{-2} has been achieved for the PEDOT:PSS film after post-treatment with 10 % Na_2SO_3 in the DMSO/salt mixture (v/v), outperforming $NaHCO_3$. The initial DMSO-doping treatment induces a distinct phase separation by facilitating the aggregation of the PEDOT molecules. At the same time, the subsequent DMSO/salt de-doping post-treatment strengthens the selective removal of the surplus non-conductive PSS chains. Substantial alterations in the oxidation level, chain conformations, PEDOT crystallites and their preferential orientation are observed upon treatment on the molecular level. At the mesoscale level, the purification and densification of PEDOT-rich domains enable the realization of inter-grain coupling by the formation of the electronically well-percolated network. Thereby, both electrical conductivity and Seebeck coefficient are optimized[3].

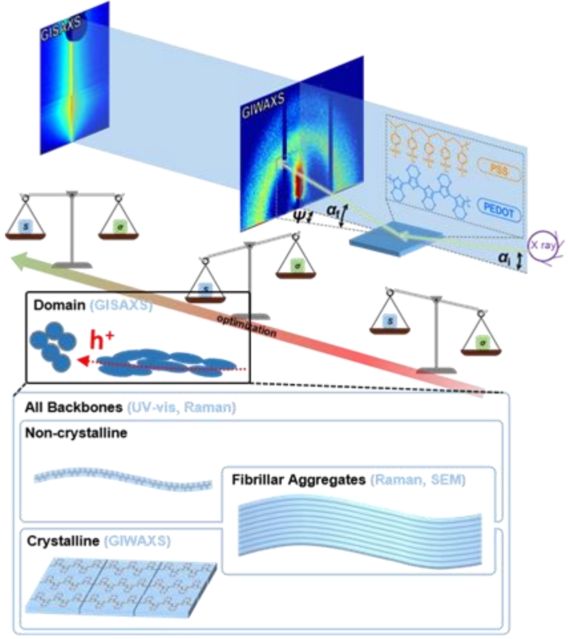

Figure 1: Schematic diagram representing the enhanced mechanism for PEDOT:PSS films.

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Morphology control of block-copolymer directed mesoporous ZnO thin films via slot-die coating

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Mesoporous ZnO thin films have received tremendous attention in photovoltaic applications in view of their high electron mobility, high transparency, high surface area, and superior ability to host the light-harvesting dyes and the organic molecular hole-transporters [1,2]. Considering the morphology-dependent device performance, precise control over the ZnO nanostructures is indispensable. Among the existing synthesis routes, the diblock copolymer-assisted sol-gel approach has been corroborated to be powerful and promising in morphology tunability [3]. Benefiting from the solution processability, this wet chemical method can be integrated into industry-based processes and thus achieve large-scale, high-throughput production. In the present work, an amphiphilic diblock copolymer is used as the structure-directing agent and slot-die coating is applied as the deposition technique to fabricate the mesoporous ZnO films. Effects of ZnO precursor variables on the morphological evolution of mesoporous ZnO films are systematically investigated. The generated nanostructures on the film surface are detected by a surface-sensitive scanning electron microscope (SEM), and the inner morphologies are probed by reciprocal-space Grazing-incidence small angle X-ray scattering (GISAXS) technique.

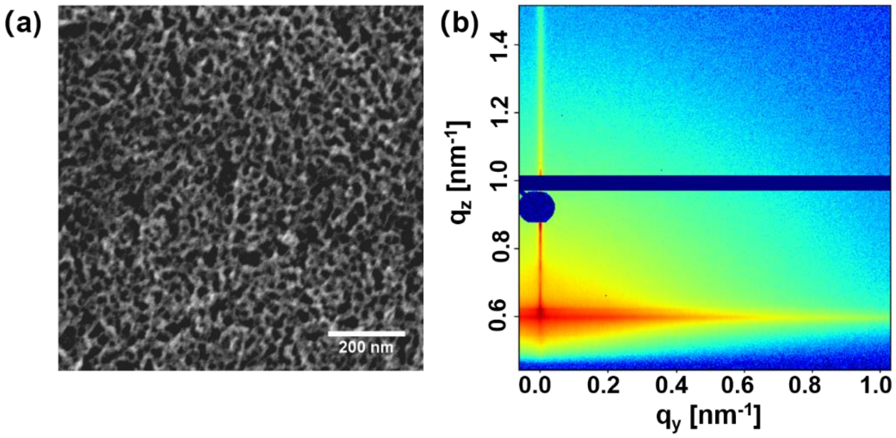

Figure 1: a) SEM image and b) 2D GISAXS data of printed mesoporous ZnO film after template removal.

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A Space Experiment for Novel Solar Cell Technologies

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The emerging thin-film photovoltaic technologies based on perovskite and organic materials are becoming more and more interesting for commercialization. Towards their application in space, flexible and thin modules that are ultra-lightweight are highly interesting.

So far, performance data of their behavior in space environment is very limited. Besides promising laboratory experiments that can never capture the full set of ambient conditions present in space, some near-space experiments have been performed in the upper atmosphere with appealing results regarding the performance and stability of the novel technologies.

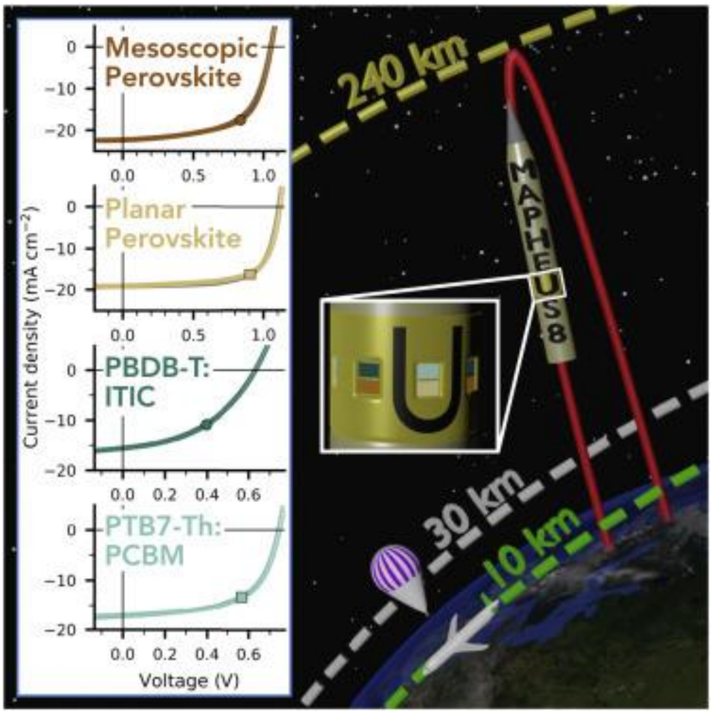

Figure 1: Graphical abstract giving an overview of the solar cell rocket experiment. [1]

Here we present the first electrical characterization of perovskite and organic solar cells at orbital altitudes [1]. Space flights are an ideal platform to investigate the behavior of our solar cells in conditions that are characterized by ultra-high vacuum, strong UV solar irradiation, and the absence of oxygen or water outside Earth's atmosphere. During a suborbital rocket flight, we measured the voltage-current response of our solar cells under different illumination conditions. The combination of the solar cell measurements with irradiance data obtained from simultaneous light sensor measurements allows for deducing the performance parameters of the different solar cell systems. Our results show that the solar cells survived the harsh conditions during transport, the start preparation procedure, and the rocket launch, where the solar best solar cells reached power conversion efficiencies of more than 10% for perovskite-based solar cell modules. Our results show the versatility of perovskite and organic solar cells for application in various environmental conditions, with promising potential to revolutionize future renewable energy production on Earth and beyond.

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Electrochemical Top-Down Synthesis of Nanostructured Support and Catalyst Materials for Energy Applications

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Functional nanostructures such as nanoparticles are a promising class of materials for energy applications due to their unique properties. Bottom-up synthetic routes for nanostructured materials often involve multiple synthesis steps and the use of surfactants, reducing agents or stabilizers. This results in complex and extensive synthesis protocols.[1] In recent years, a novel top-down synthesis approach to form metal nanoparticles has been established, in which bulk metal wires are immersed in an electrolyte (primarily alkali earth metal based) and subsequently subjected to a high alternating potential. This leads to erosion of the metal wires to nanoparticles dispersed in the electrolyte.[2] The main advantages of this facile top-down approach is that there are no reducing agents, surfactants or precursor solutions. The complete synthesis can be performed in one pot involving one main step with consequent washing and drying of the nanoparticles. More recent studies investigated the effect of synthesis parameters such as potential amplitude, frequency, electrolyte composition and concentration on the size and shape of the nanoparticles.[3]

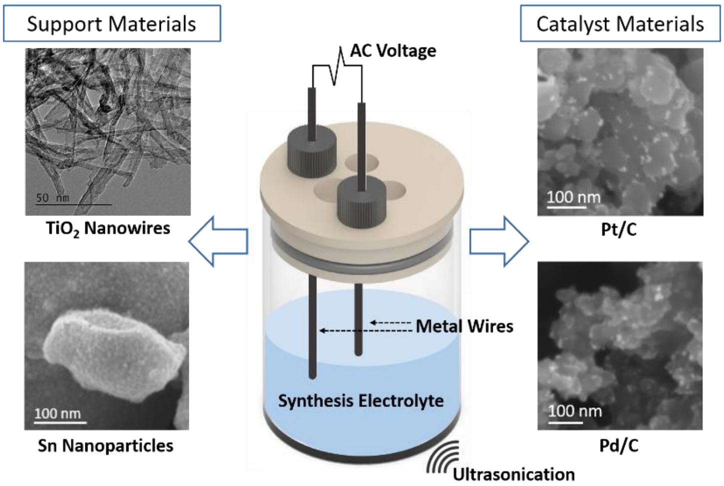

Figure 1: Schematic illustration of the electrochemical top-down synthesis of nanostructured energy materials. Application of an alternating sinusoidal potential to metal wires during ultrasonication in various types of electrolytes leads to the formation of nanostructures. This synthetic route enables the generation of catalyst materials like Pt/C or Pd/C (SEM images on the right side) as well as support materials like TiO_2 nanowires (TEM image in top left corner) or Sn nanoparticles (SEM image in bottom left corner) as alternatives to widely used carbon support materials.

Here, we investigate the electrochemical erosion of various metal wires such as Ti, Pt, Pd and Sn in various electrolyte compositions *via* this facile top-down technique and its experimental optimization to successfully synthesize nanostructured materials for various energy applications as indicated in **Figure 1**. As an example, for Pt and Pd, homogeneously distributed nanoparticles on carbon support (see SEM images on the right side in **Figure 1**) can be obtained. These materials can be used as electrocatalyst materials for the oxygen reduction reaction (ORR) and hydrogen evolution reaction (HER), respectively. Whereas the top-down erosion of Sn wires leads to the formation of nanoparticles (see **Figure 1**, bottom left), which have great potential as oxygen evolution reaction (OER) support materials. The application of the technique on Ti wires surprisingly leads to the formation of nanowires (see **Figure 1**, top left), which show a high surface area and demonstrate a great potential as an alternative support material to carbon.

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Fabrication and Characterisation of Two-step Slot-Die Coated Perovskite layers

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Solar cells are very promising in becoming one technology in the renewable energy mix of the future. There are so-called perovskites within the solar cells as absorption material with their respective ABX3 structure. X represents an anion, and A as B are cations of several sizes. Perovskite absorbers have the advantages of a high absorption coefficient, a tunable bandgap, a large dielectric constant, a low exciton binding energy, and ambipolar charge carrier mobilities. Furthermore, do Perovskite Solar Cells (PSCs) have high power conversion efficiencies and are made of low-cost materials. Further aspects can be found in [1].

Especially in combination with slot-die coating as promising thin-film deposition technique for organic-inorganic hybrid perovskite materials. [2] Figure 1 shows a slot-die coater, which is printing a PbI2-layer.

In this work, two-step slot-die coated lead iodide (PbI2) and slot-die coated methylammonium (MAI), and methylammonium-formamidinium (MAI-FAI) iodide perovskite layers were produced. The advantages of two-step slot-die coating are not handling the same solvent for all precursors, more chemical flexibility, easier orientation tuning of the final perovskite crystals, and more control during the film deposition process. Further information can be found in [3].

Figure 1: Slot-Die coater printing a PbI_2 layer

For the first printing step, lead iodide is dissolved in a solution and its deposition depends on slot-die parameters and additive. An additive tunes the bandgap and enhances the thin film-formation and optoelectronic properties of the final perovskite semiconductor absorber. Furthermore, morphology changes are observed. These are investigated by reciprocal (e.g., X-ray diffraction) and real-space methods (e.g., SEM). A solvent containing MAI and 2-propanol (IPA) is printed on top of the first layer and perovskite is formed within the second printing step, as shown in Figure 2.

Figure 2: Two-step printed $MAPbI_3$-perovskite layers

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Supply concept for multiple use of renewable energies

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At Hof University of Applied Sciences, a supply concept with various applications of renewable energy (RE) is currently under development as part of the new building - the Institute for Water and Energy Management (iwe). The integration of multiple RE into the entire building-concept represents an innovative and promising approach towards achieving future energy goals, especially in the decentralized sector. The idea is not only to activate a large area of the buildings envelope in terms of energy, but also to integrate other solutions for conversion and storage in as well as around the building to increase autarky. In order to ensure a more efficient use of fluctuating RE, solutions for demand-optimized storage and management of their different inlet temperatures are required. For this purpose, the stratified storage technology has been proven particularly suitable. Flow-optimized loading devices and intelligent control of the heat sources, some of which occur simultaneously, can additionally increase overall efficiency by minimizing internal turbulence.

Figure 1: Side view iwe incl. thermal collectors [von M GmbH]

Air-to-water and brine-to-water heat pumps, solar thermal energy, wind energy, photovoltaics and coupled photovoltaics-thermal energy solutions are being integrated into the overall building concept. The modularly adaptable facade concept includes the integration of thermal collectors into a circumferential shading concept (see figure 1). The unpressurized large thermal energy storage tank with more than 40 connections to the building hydraulics is centrally placed and has a capacity of approximately 150 m³ (see figure 2). The stratified heat storage enables efficient control of all heat flows in the building and thus serves as a central element for optimized building control. Flow- and application-optimized loading and unloading devices such as stratified charging lances, radial and linear diffusers, ensure efficient operation by reducing internal turbulence. In addition to the storage of pure thermal energy, sector coupling is enabled by the use of surplus electric RE by means of heat pumps and electric heaters. Since the building is to serve as a research platform, other energy-research facilities, such as micro-CHP's, ice storages and laboratory machinery, are also coupled to the stratified storage tank via predefined interfaces and can thus additionally contribute to the overall energy supply of the building. With its high local resolution, an integrated fibreoptic temperature measurement (“distributed temperature sensing”) allows for detailed monitoring and accurate validation of the flow processes inside of the storage tank. One will initially work with a commercial building control system. However, research activities are planned to exploit the possibilities of a predictive control system.

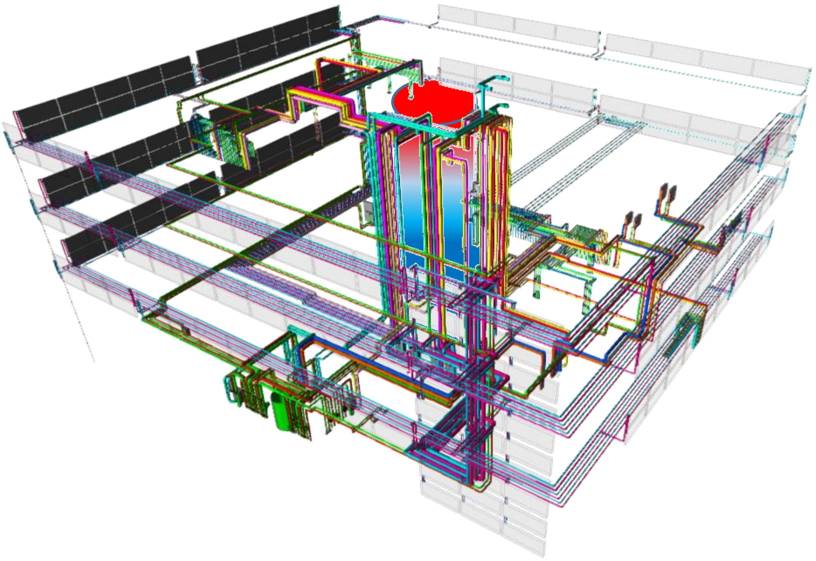

Figure 2: Hydraulic system for use of RE incl. stratified heat storage tank [H + S ingenieure GmbH]

Mitigation of Contact Resistance Formation in Proton Exchange Membrane Water Electrolyzers during Intermittent Operation

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Proton exchange membrane water electrolysis (PEMWE) is a promising technique to produce “green” hydrogen when coupled with fluctuating renewable energy sources. Since water electrolyzers require a long lifetime to reduce cost per kilogram of hydrogen, degradation mechanisms of the different materials and components in the cell have to be investigated, so that conditions causing the degradation can be avoided.[1] Therefore, accelerated stress tests (ASTs) have been developed to enable efficient material screening and identification of failing and degradation mechanisms on a shorter timescale.

Weiß et al.[2] conducted ASTs mimicking intermittent operation of a PEM water electrolyzer with idle periods. The test protocol consisted of cycles comprising steps at current densities of 3 A/cm^2 and 0.1 A/cm^2, followed by an idle period at open-circuit voltage (OCV), which was repeated for more than 700 cycles. The authors attributed the major fraction of the observed performance losses to the passivation of the titanium porous transport layer (PTL) on the anode in combination with a reduced conductivity of the anode catalyst layer. In order to mitigate the formation of an insulating oxide layer on the PTL they suggested applying a gold surface coating to the PTL.[2] However, a recent study by *Liu et al.*[3] revealed that an Au-coating on a Ti-PTL is not sufficiently stable under operating conditions on a timescale of 4,000 h. The authors therefore proposed the use of Pt- or Ir-coated Ti-PTLs.

This study aims to mitigate the formation of a contact resistance between the PTL and the anode catalyst layer of a PEM water electrolyzer during intermittent operation by using a Ti-PTL with a noble-metal coating. Measurements are performed in a 5 cm^2 PEMWE single cell with an IrO_2/TiO_2 anode catalyst. The protocol of *Weiß et al.*[2] is employed with the addition of cell diagnostics at 1.3 V after the OCV-period (fig. 1). This poster presents a comparison of the OCV-ASTs conducted with a Ti-PTL, resulting in an increasing high frequency resistance (HFR), and a Pt-coated Ti-PTL, yielding no increase in HFR and therefore, no contact resistance formation. Thus, the use of a Pt-coated PTL is suited to investigate degradation phenomena of a PEM water electrolyzer without superimposed contact resistances.

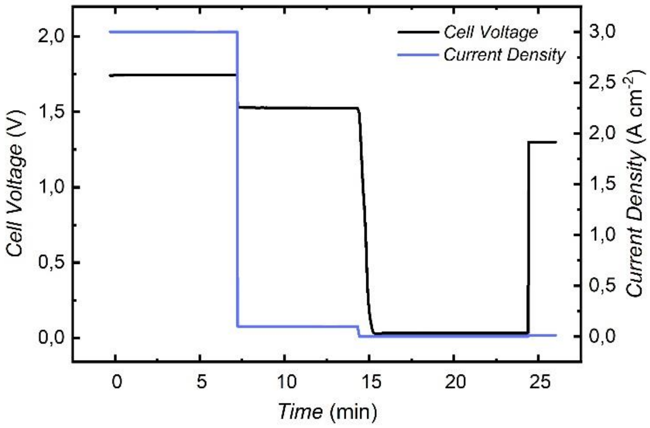

Figure 1: Cell voltage and current density profile of one OCV-AST cycle.

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Enabling long-term investments in low-carbon energy systems in South America through joint interregional energy system planning

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South America is a fossil fuel producer and global supplier, with countries exporting large amounts of its production of gas, coal, and petroleum, therefore making their economies highly dependent on the fiscal revenues that these exports bring [1]. This study is centred around the electric systems of Colombia, Ecuador, and Peru; these countries have different approaches on their energy policies, Peru for example relies 50% on hydropower and 50% on fossil fuels for electricity production, while Ecuador and Colombia rely mostly (>70%) on hydropower electricity and they complement with their own fossil production. One common ground for all the countries is the decline in the electricity trade as they secure their electricity needs internally [2].

Figure 1: Modeled Nodes; Colombia green), Ecuador (blue) and Peru (purple)

The evidenced negative effects of carbon emission on the global climate and society demand a transition to an energy production that is both cost-efficient and environmentally friendly. Fortunately, there is an abundance of solar, wind and hydro resources in the studied countries that create the opportunity to diversify the generation matrix by using renewable resources and achieve simultaneously the reduction of the carbon emissions. These three countries have ambitious plans for renewable electricity systems but at the same time the economic dependency on the exports of non-renewable sources keeps fuelling several investments of fossil fuel exploitation. Achieving a large renewable energy penetration into the regional energy system requires to understand the potential for renewable energy generation in the studied countries as well as the opportunities that an international market between the countries could create.

This study applies the linear programming cost-optimization model *urbs* to evaluate collaborative and non-collaborative long-term investment for renewable power generation in Peru, Ecuador and Colombia. The model *urbs* explores future energy system configurations for the planning horizon 2019-2050, considering also an hourly spatial resolution which captures the variability of renewable energy sources. The objective is to assess future investment trajectories in renewable capacity expansion with different levels of cooperation between the countries for Ecuador, Peru, and Colombia by minimizing the net total costs of the investment and operating costs of the entire energy system. Furthermore, scenarios that reflect the variability of the hydropower electricity generation are evaluated. The resulting energy configurations are assessed and compared by their costs and ability to secure power supply.

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Investigation of the Chemical Delithiation of Ni-rich Layered Oxides

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Combatting climate change necessitates the reduction of carbon emissions. Hence, new ways of energy storage aside from volatile fossil fuels must be adapted. The lithium-ion battery (LiB) is a suitable candidate with high energy density and is especially viable in weight and size-constrained applications. However, for successful employment, the long-term stability must be improved, guided by fundamental insights into the various material aging mechanisms. In order to deconvolute deleterious aging mechanisms, stability analysis of the cathode active material without complex matrix influences from the LiB-assembly is necessary. Utilizing a chemical extraction of lithium from these materials would result in large quantities of raw material (powder) at various degrees of delithiation.[1] Upon delithiation, the layered structure of these materials is destabilized, causing oxygen release and phase changes within the material upon subsequent heat-treatment. The resulting partially oxygen depleted material mimics CAMs within a LiB, which have undergone extensive electrochemical cycling. The onset temperature and the amount of released gas can further be utilized as semi-quantitative predictors for the long-term stability of CAMs, avoiding costly and lengthy long-term testing.[2]

Here, we evaluated the process of the chemical delithiation in comparison with the electrochemical delithiation of Ni-rich CAMs.[3] Previous studies have shown proton insertion in chemically delithiated CAMs.[4] Hence, we assessed our setup for the reduction of trace water during the chemical delithiation. We focused on state of the art Ni-rich $Li_1Ni_{0.8}Co_{0.1}Mn_{0.1}O_2$ (NCM811) as CAM due to its commercial importance and high energy density within a conventional operation potential window.[5] After chemical delithiation, the material retained its crystalline structure and electrochemical behavior. Reaching low lithium contents, however, the chemically delithiated material experienced phase separation into two discrete layered phases. This phase separation has been observed in electrochemically cycled NCM811 and is attributed to strain on parts of the layered structure during the contraction of the crystal lattice at high degrees of delithiation.[6] The build-up of a resistive phase was further observed in galvanostatic cycling analysis by increasing polarization. The weight loss upon heat-treatment corresponds to the decomposition of the delithiated material into a fully lithiated layered and a rock-salt phase, also observed in the surface-region of electrochemically aged Ni-rich NCMs. This decomposition for the chemically delithiated materials is accompanied by the release of oxygen and water, with the water originating from inserted protons into the material. Chemical delithiation was found to alter specific chemical and physical properties of the material of interest, in ways similar to extensive electrochemical aging, however, in a more pronounced fashion. The chemical delithiation can access bulk quantities of destabilized materials for an isolated analysis of degradation pathways and its decomposed crystal phases in the material and can provide deep mechanistic insights. It further provides a fast tool to optimize and screen new materials for their respective properties. However, the information gained from this procedure must be assessed critically in context of its formation.

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Investigation of Na^+ diffusion in NASICON solid electrolyte materials by Quasi-Elastic Neutron Scattering

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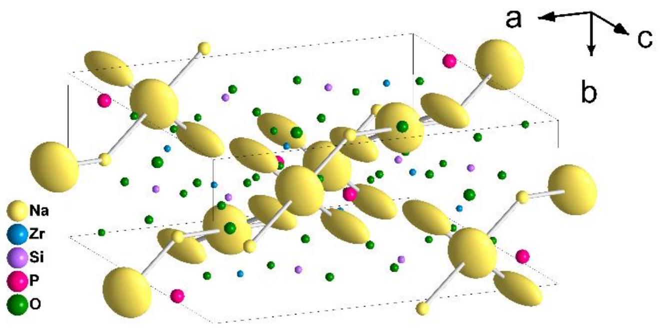

Figure 1: Monoclinic structure of NASICON with possible positions for Na diffusion (yellow) in the crystal structure

In the recent years, sodium superionic conductor (NASICON) materials have been a widely studied class of solid electrolytes for Na-ion based all-solid-state batteries due to their high conductivity and facile synthesis conditions [1]. The aim of this work is to clarify the reason for extremely high conductivity exhibited by some compositions, specifically by $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ ($0 \leq x \leq 3$). The focus of this study is to explain the role of the monoclinic to rhombohedral phase transition for the material with x=2.4, which occurs at around 170 °C, on the Na^+-ion occupancy and diffusion in the crystal structure. Additionally, we investigate the role of Al/Y and Sc substitution on Na+-ion mobility and the overall temperature dependence of the ionic conductivity in the temperature range of 297-640 K. We can see a structure model of one of the NASICON structures $Na_{3.4}Zr_2Si_{2.4}P_{0.6}O_{12}$ in Figure 1. Yellow ellipsoids indicate the possible diffusion paths for Na diffusion in the crystal structure. In general, neutron scattering techniques are highly suitable for measuring the properties of crystalline materials. Here, quasi-elastic neutron scattering (QENS) is applied to measure the spatial and temporal dynamic properties of diffusion of Na^+ ions in the crystal lattice. This technique is feasible, because sodium is the only diffusive element in the material and the only one scattering incoherently. The measurements were performed at the BASIS spectrometer at the Spallation Neutron Source, Oak Ridge National Laboratory in Tennessee, USA. For the evaluation of the QENS data, the DAVE software is used [2]. The Na^+-ion diffusion mechanism can be described by the right choice of the diffusion model, in this case the Chudley-Elliott jump diffusion model has been used. In Figure 2, we can observe an example of the collected QENS spectra. The QENS data are measured at different temperatures and different scattering vectors Q. Each spectra is fitted with a background function, delta function and two Lorentzian functions. The two Lorentzian functions describe two different diffusion process – local and long-range diffusion. Important parameters, such as diffusion coefficients, activation energies, jump distances between the occupation sites and residence times are extracted from the measured and modelled QENS data.

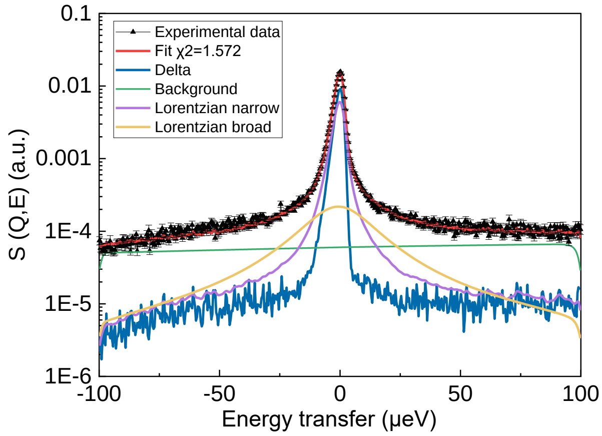

Figure 2: An example of fitted QENS spectra at 400 K and Q = 0.7 Å^{-1}

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Silicon-Germanium based anode coatings for Lithium-ion batteries

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Because of irreversible damage to the climate and human health caused by fossil fuels and unreimbursed input of energy from the earth to human activities, the generation and storage of renewable energy is an urgent challenge for humankind.

In this regard, lithium-ion batteries (LIBs) have drawn increasing attention over several decades as an indispensable role in energy storage. To further optimize the performance of LIBs, Si with a theoretical capacity of 4200mA h g^{-1} ($Li_{4.4}Si$)[1], high abundancy, and an appropriate on-set potential of 0.4V[2], has been intensively investigated since the 1990s. However, the application of silicon on anodes is hindered by the volumetric expansion (360%) after full lithiation, which causes collapse with three failure mechanisms including electrode pulverization, the disconnection between the electrode and current collector, and continuous breaking and re-growth of the solid electrolyte interface (SEI) layer[3]. To tackle this critical issue, the construction of the hierarchical structures i.e. physical compartment contributes a promising way to increase the stability of active materials.

In our studies, Si/Ge hierarchical structures are built by chemical templating of pre-nanostructure self-assembled by PS nanoparticles, and using an amphiphilic polystyrene-*block*-polyethylene oxide (PS-*b*-PEO) diblock copolymer as a structure-directing agent. The diblock copolymers undergo microphase separation by their property of self-assembly[4], which is also further modified by solvent vapor annealing[5] with dichloromethane (DCM) and $SiCl_4$. By pyrolysis, mesoporous thin films are achieved. The desirable morphological and crystallographic studies are accomplished by grazing-incidence small-angle X-ray scattering (GISAXS), SEM, AFM, and grazing-incidence wide-angle X-ray scattering (GIWAXS). The study is completed by galvanostatic cycling tests and impedance spectroscopy.

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Influence of cooperation and flexibilities in the future transformation of distribution grids – a MILP approach

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In addition to electricity, decarbonization of heating and mobility is essential for a consistently sustainable energy future. Large-scale electrification of these sectors, especially at the household level, appears to be a promising goal for many countries, as it allows a) the use of local, scalable renewable energy technologies such as photovoltaics (PV) and wind energy, thereby reducing dependence on fossil fuel imports, and b) the use of high-efficiency technologies such as residential heat pumps and battery electric vehicles (BEVs). Traditional distribution grid planning, while oversized, was were oversized to some degree, did not anticipate a level of electrification that would meet current decarbonization goals. In addition, residential heating is associated with higher simultaneity than conventional electricity demand as its use is generally correlated with lower ambient temperatures. Therefore, large-scale adoption of these technologies by households in the future will cause significant reinforcement needs in the distribution networks.

In this work, a mixed-integer linear programming approach is introduced to explore a global optimum that can be achieved through simultaneous co-optimization of distribution grid reinforcement and flexibility measures. The coverage of electricity, heat and mobility demands is considered. Since the optimum achieved by the MILP approach represents a single social planner that minimizes a single cost function for the entire system, it inherently assumes the full cooperation of all agents in the system, i.e., residential customers and the distribution system operator. Since such system planning and operation is far from practical under the current regulatory framework, these results are then put into perspective by the implementation of more realistic, albeit suboptimal, planning schemes. Through this comparison, the value of flexibility components and cooperation between actors in distribution networks is quantified.

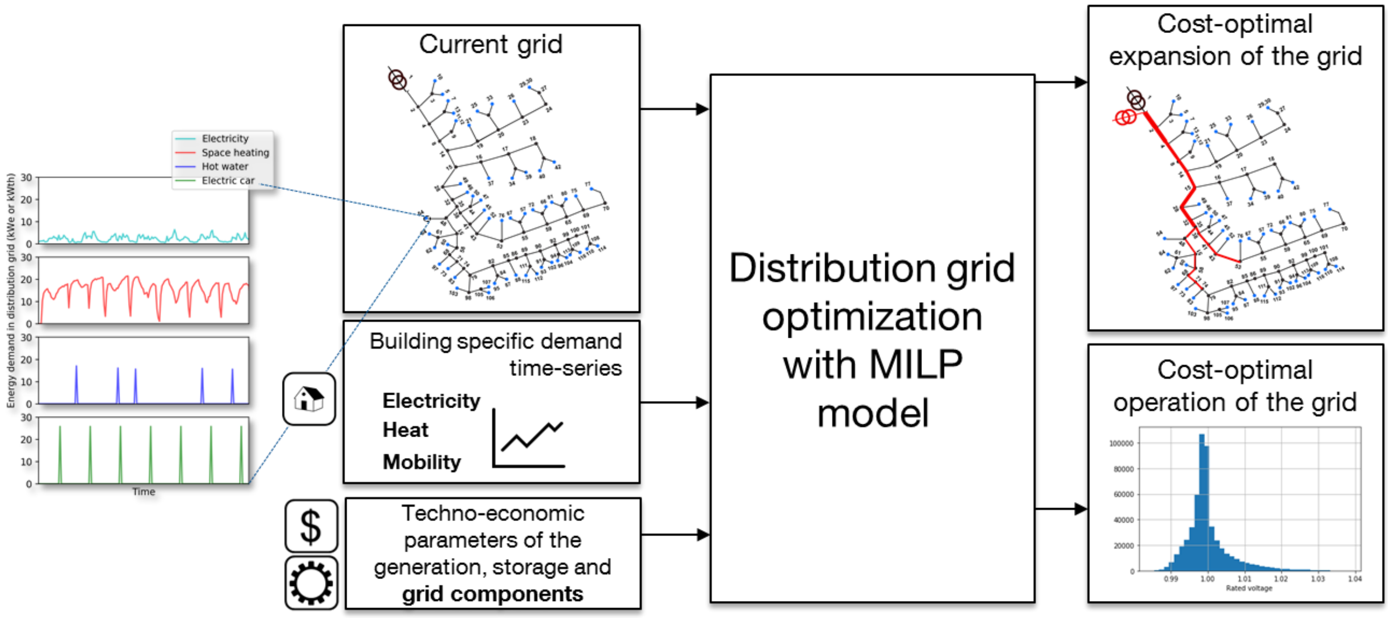

Figure 2: Sector-coupled distribution grid capacity expansion and operation framework.

Printing of perovskite quantum dot layers for solar cell application

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Figure 1: Different Perovskite quantum dots under Ultraviolet (UV) light [1]

Perovskite quantum dots solar cells (PQDSCs) are one of the promising new generation solar cells that have gained tremendous interest in the last few years. Due to their exceptional properties such as tunable bandgap, high defect tolerance, and good stability, they are promising candidates. PQDSCs are based on perovskite quantum dot (PQD) layers, where the light gets absorbed, and excitons are generated. The excitons are separated in the device and the resulting electrons/holes can be used as electrical power. PQDs or nanocrystals (NCs) are semiconductor nanoparticles of the form ABX_3, where A represents a cation (organic like formamidinium (FA^+) or inorganic like cesium (Cs^+)), B is a lead cation (Pb^{2+}), and X is a halide anion (bromide (Br^-), iodide (I^-) or chloride (Cl^-)), which gives PQDs their outstanding optoelectronic properties (see Figure 1). Nowadays, PQDs are mainly synthesized by the hot injection (HI) method, a simple procedure that allows for scalable synthesis and allows tuning the size of the QDs by temperature variations. To prevent the synthesized PQDs from aggregating together and losing their properties, they are enclosed with different ligands such as oleic acid (OA) and oleyamine (OAm) (see Figure 2).

Currently, PQDSCs are mainly fabricated using the spin coating technique, which has proven to be very successful in recent years. However, due to the large amount of waste generated by spin coating, other approaches are needed for scalable PQDSCs manufacturing. The slot-die coating technique represents one of the successful techniques that significantly reduces waste and has already been used to print several new types of solar cells, such as organic or bulk perovskite solar cells. The key component of the slot-die coater is the slot-die head, which delivers the required amount of solution directly onto the substrate, so that almost no solution is wasted.

In this work, we develop printing of PQD layers using the slot-die coating technique and compare them with spin coated layers. To study these layers, we use various techniques such as UV-vis, scanning electron microscopy, X-ray diffraction, photoluminescence.

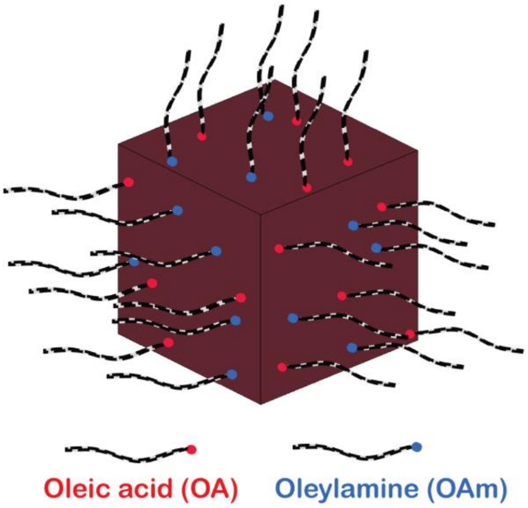

Figure 2: Schematic representation of a perovskite quantum dot surrounded by OAm and OA ligands.

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Sustainable and profitable energy system development in Bosnia and Herzegovina

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Climate change and agreements on greenhouse gas emission mitigation force a transition of energy production to more sustainable and efficient technological solutions. However, in contrast to most EU countries, governments across southeast Europe plan to build new lignite power plants during the next few years [1, 2]. Lower electricity costs, especially important because of poor economy and purchase power of the region, shift weight towards fossil fuel usage. With the background of global air pollution reduction goal, the energy system of Bosnia and Herzegovina is possibly offering a low-hanging fruit, for which a decarbonized and profitable future development can be found.

The goal of this work is to investigate the cost optimal solution for Bosnian energy system development and trends which would support a more sustainable energy sector. Current state of the system, energy demand progression, various price trends, political changes like global CO2 certificate market, and eventual restrictions on extension of renewable power plants are to be considered. Currently, about two third of the country's electrical energy is generated in coal power plants, while the remainder is coming from hydropower, and marginally wind and solar generation capacities [3]. The coal prices in the region are much lower in comparison with the European average [4]. Additionally, already existing expertise in extension and operational planning of this power plant type favors it in comparison to jet rather new technologies. The electricity system of Bosnia is in this work observed on multiple levels. First as an isolated system and secondly as a part of the European electricity system. Through the scenario analysis it can be concluded, what are the most cost-effective development solutions in Bosnia and Herzegovina which fulfill the goal of a sustainable development. Furthermore, we can deduct, how this development can be supported and what chances does a global system planning offer.

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Structural Peculiarities of Co-precipitated Ni-Al Catalysts for CO_2 Methanation

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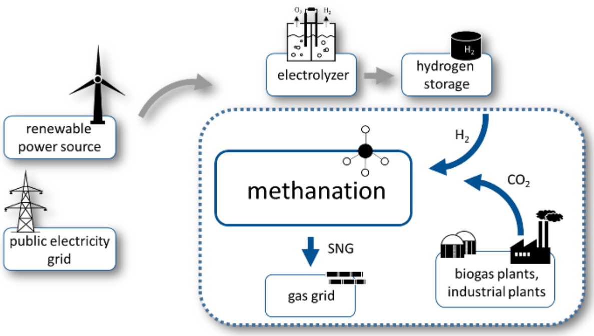

Figure 1: Methanation in the context of the power-to-gas (PtG) concept.

Regarding global warming, effective methods of storing energy from sustainable sources are becoming increasingly important. The so-called power-to-gas (PtG) concept is a much-noticed approach in this context. Hereby, the energy from renewable sources is converted into hydrogen *via* electrolysis of water and is then converted with CO_2 into methane as part of the so-called methanation.[1] To produce methane effectively, highly active, selective, and stable catalysts are needed.

Co-precipitated Ni-Al materials meet all these requirements and are an excellent choice as methanation catalysts. However, their exact structure has not yet been clarified. For that purpose, we synthesized catalysts with different Ni/Al ratios ($n_{Ni}/n_{Al} = 5 – 0.33$) which were calcined in synthetic air and activated under H_2 atmosphere. The materials were characterized in detail in their co-precipitated, calcined, and reduced states.

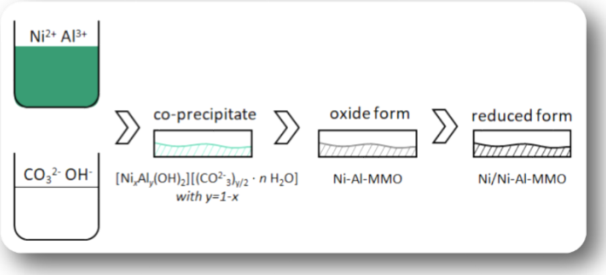

Figure 2: Different stages in the preparation of co-precipitated Ni-Al catalysts. Adapted from [2].

Directly after co-precipitation, the materials feature a hydrotalcite-like structure, showing an increasing basal interlayer distance with rising Al content. After calcination at 450 °C, this structure is transformed into a Ni-Al mixed metal oxide (MMO). The decomposition occurs *via* the release of H_2O and CO_2 stemming from water and carbonate molecules located in the brucite-like interlayers and condensation of the hydroxyl groups in the brucite-like layers of the co-precipitate. In this state, a Ni-rich crystalline phase coexists with an amorphous alumina-rich phase. In the crystalline phase, Al^{3+} ions are incorporated into a fcc NiO structure which leads to a distortion of the unit cell depending on the Al content. A detailed XRD study using Rietveld fitting showed that, in addition to the mixed oxide phase, the sample also contained a certain proportion of uncalcined precursor residues. A dependency of the proportion of these residues in the examined sample on the existing aluminum content could be determined. In principle, in this material Al serves to ensure the temperature stability of Ni, which is susceptible to sintering. Reduction of the Ni-Al mixed metal oxides leads to formation of two different phases, an elemental Ni phase and Ni^{2+}-containing aluminum oxide-rich phase. At high aluminum contents, an additional amorphous alumina phase is assumed. In comparison, samples with high Al content featured a hampered reducibility which could be traced back to the structural deviations in the oxidic material. A possible consequence could be aluminum-containing inclusions in the Ni crystallites.

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Revisiting the active surface of $Cu/ZnO/Al_2O_3$ catalysts for the methanol synthesis

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The mitigation of climate change plays a key role in today's society with the CO_2 hydrogenation to methanol being a powerful tool to reduce the usage of fossil fuels. With an annual production of around 98 Mt methanol has a very important role in the chemical industry and as an emerging energy fuel. While still mainly produced from fossil sources the production of renewable methanol from waste CO_2 and sustainably derived hydrogen can be an efficient way towards net carbon neutral goals and to store and transport energy from renewable sources. Even though $Cu/ZnO/Al_2O_3$ catalysts are used for industrial methanol synthesis for more than 50 years, the nature of the active site and the reaction mechanism are still under constant debate and investigation. In this study, we combine quasi *in-situ* X-ray photoelectron spectroscopy (XPS) with measurements in a standard lab-scale reactor setup to shed light on the composition of the surface of an active catalyst under operating conditions while closing the pressure gap.

A co-precipitated $Cu/ZnO/Al_2O_3$ powder catalyst was analyzed under various experimental conditions in a reactor setup (conditions: -196 °C – 300 °C, 1 bar – 25 bar) using Temperature Programmed Desorption (H_2-TPD) and Reactive Frontal Chromatography (N_2O-RFC) and in an ultra-high vacuum (UHV) chamber equipped with a XP- and a mass spectrometer (MS). The UHV setup consists of a 'high-pressure cell' ($\leq$ 1 bar) directly attached to the XPS analysis chamber allowing quasi *in-situ* measurements of an active catalyst as confirmed by MS. In both setups, the gas phase composition (H_2, CO, CO_2), overall pressure and temperature can be adjusted as needed.

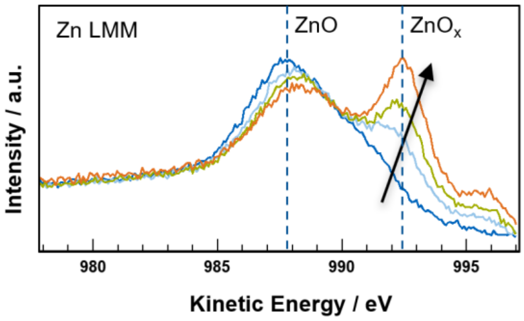

Fig. 1: Zn LMM Auger spectra upon proceeding reduction.

First, the activation in H_2 at different temperatures of a calcined catalyst precursor was analyzed in both setups. Using XPS, the complete reduction of Cu^{2+} to Cu^0 was observed, while Zn remained entirely as ZnO at 175 °C. Upon further reduction at 240 °C, a shoulder in the Zn LMM Auger spectrum starts to form indicating a partial reduction of Zn^{2+} surface species. The shoulder gets more pronounced with increasing temperature (*cf*. Fig. 1). A significant decrease in the Cu 2p/Zn 2p ratio reveals that metallic Cu particles are formed at first, followed by the formation of a ZnO_x layer over the Cu particles at 240 °C as also postulated by Fichtl et al. [1]. These findings were compared to the transient measurements, which also confirm the formation of a ZnO_x overlayer.

To analyze a catalyst under operating conditions, a feed gas with the stoichiometric composition of $CO/H_2 = 1/2$ was chosen due to the thermodynamics of the methanol synthesis at 900 mbar. This enables us to produce methanol in a UHV setup and consequently monitor the surface of the active catalyst by XPS. The Cu and Zn core level spectra showed no difference to the ones obtained after activation indicating that the surface after activation is also the catalytically active one. As no changes in the Cu signals were observed upon the reaction, the oxidation state and particle shape stayed the same. Also, partially reduced Zn species were found on the surface of the active catalyst.

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Technical and economic analysis of waste heat recovery systems based on the organic Rankine cycle (ORC) for marine Diesel engines

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ENGIMMONIA, an EU-funded project, intends to decarbonize long-distance shipping by investigating Ammonia as a clean fuel for the shipping sector and by examining multiple energy efficiency technologies that can be implemnted on large-scale vessels. Organic Rankine Cycles (ORC), adsorption chillers, and photovoltaics (PV) will be coupled with an energy management system (EMS) and installed on-board the demo-vessels of this project, including a Very Large Crude Carrier (VLCC), a container ship and a ferryboat. These technologies have the potential to reduce future GHG emissions and might be useful for future cargo and passenger transportation in the maritime industry. This work highlights the ORC potential in this project.

The ORC can use the waste heat available from the exhaust gases of the ship's Main Engine (ME) directly or from the steam generated by the Exhaust Gas Economizer (EGE). It can also make use of waste heat available from the Jacket Cooling Water (JCW) of the ME to preheat the working fluid of the ORC. The energy output of the ORC system is converted into electricity to supply the on-board grid. Utilizing the JCW for preheating allows for greater power generation, which reduces auxiliary engine fuel consumption and increases ORC feasibility [1]. **Figure 1** shows the layout of the ORC system, with heat recovered from both the EGE's steam and the JCW.

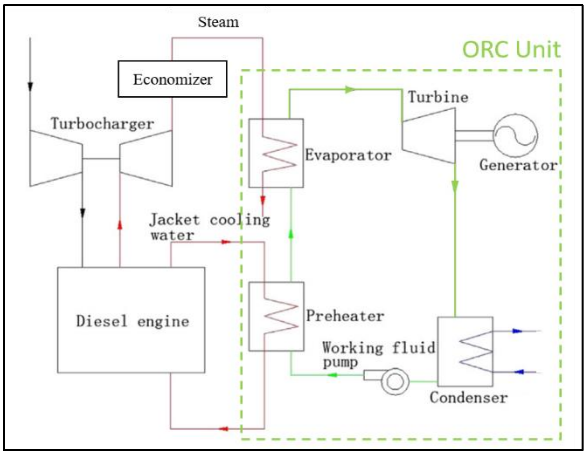

Figure 1: ORC layout from recovery

The current model developed to estimate the potential of the ORC system in this project shows that the ORC technology is an attractive investment with a positive Net Present Value (NPV), when it is operated for at least 10 years and there is a fixed amount of excess steam available for the ORC utilization. However, this is not the actual case for many vessels. Consequently, In order to increase the accuracy of the model, a more accurate steam profile will be developed at a further stage with the help of operational data obtained from the EMS installed on-board.

The ORC feasibility strongly depends on the fuel prices, The ORC's economic potential is adversely affected by lower fuel prices. It also depends on the available waste heat, which changes significantly with different operational modes of the vessel and different weather conditions [2]. Once the ORC is installed on-board, it will be monitored for a year. The actual data from the ORC's operation will be collected using the EMS on-board. This will provide data for validating the simulation models and it will give insight into expected and unexpected challenges when integrating the ORC on-board large-scale vessels.

Acknowledgments

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OpEn Farming: Optimizing the Energy System Vertical Farming

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The food industry undergoes major changes, and this transformation process needs to face global challenges: climate change and weather extremes, food security, water demand, nitrogen input into nature as well as reliance on phosphate and fossil fuels or the competition between cities and agricultural land. For the nexus energy-water-food, energy demand is predicted to increase by 50% and similarly water demand by 30% in 2030. Discussions are underway regarding sustainable nutrition through innovative concepts and weather independent cultivation of products under optimal conditions for plants regarding illumination, temperature and CO_2 content. This cultivation method enables a high level of control on the product, but requires huge expertise to produce high quality while using resources most efficiently. In this context, vertical farming is defined as stacked levels for optimal usage of the floor area. The main advantages here are food security and environmental protection. However, vertical farming concepts are reviewed critically since the energy demand, costs for illumination and air conditioning cannot compete with outdoor cultivation or greenhouses for the time being.

Figure 1: Growing food in optimal conditions throughout the year. Credit: Applied Science Center for Smart Indoor Farming at HSWT.

Figure 2: Vertical Farming Box. Credit: H. Kleeberger, ENS TUM.

The project OpEn Farming: Holistic Optimization of the Energy System Vertical Farming by Integrating in a Cycle Economy has been funded in 2021 by the German Federal Institute for Building, Urban Affairs and Spatial Research on behalf of the German Federal Ministry of the Interior, Building and Community with funds from Future Building (Zukunft BAU) research funding. The interdisciplinary and international research team has devoted its mission to approach the central research question, whether vertical farming has the potential to become a sustainable system for urban food production and an enabler to future agriculture.

The topics comprise:

- Developing building concepts for vertical farming, which are energetically optimized, but also economically attractive
- Integrated modeling of thermodynamic processes at plant level and the interaction with artificial illumination
- Integrating vertical farming into an extended energy system of a heterogeneous structure such as a campus
- Implementing a life-cycle-analysis optimization for vertical farming as a whole system

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aufgrund eines Beschlusses des Deutschen Bundestages

Hybrid Energy Harvester based on the Combination of Triboelectric Nanogenerator and Solar Cell

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Developing clean energy techniques lies in the heart of sustainable development of human society [1], in which collecting solar energy is one of the most promising ways in replacement of conventional used fossil fuels. However, the daily and seasonal fluctuations limit the continuous electricity generation from solar cells. Thus, integrating solar cells with other kinds of energy harvesters in one device is considered as an effective solution to provide an energy source continuously. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvester for harnessing ambient mechanical energy based on the coupling of triboelectrification and electrostatic induction effect. Compared with other counterparts, owing to its advantages of light-weight, low-cost, and easily fabricated, different kinds of TENG devices have been fabricated for harvesting various energies in the past years [2].

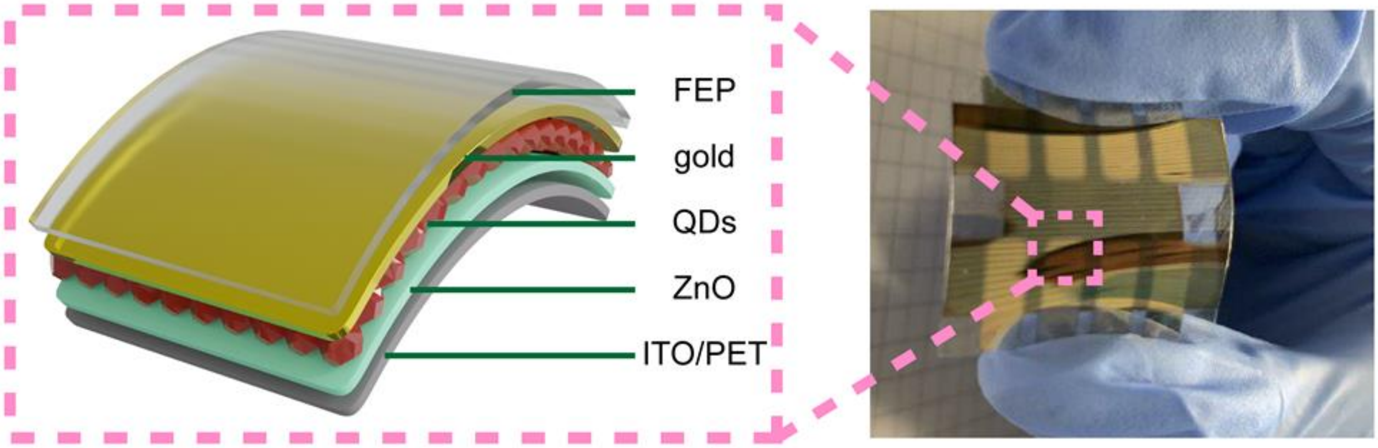

Figure 1: (left) Fabricated hybrid energy harvester as sketch and (right) in reality.

In the present work, a flexible hybrid energy harvester is designed and fabricated based on PbS quantum dots (QDs). This device consists of a QD solar cell component and a fluorinated ethylene propylene (FEP) based single-electrode mode TENG component, which can harness both, solar and mechanical energy from ambient environment to generate electricity. The structure of the hybrid energy harvester is schematically shown in Figure 1 (left). Here, the gold electrode serves as both the electrode for TENG and the anode for PbS QD based solar cell. Figure 1 (right) shows a photograph of as-fabricated energy harvester device at bending state. Additionally, grazing incidence small angle X-ray scattering (GISAXS) measurements are used to characterize the bending stability and morphology changes of the mesoscale structure [3]. This work may have great applications in smart home systems and internet of things (IoT).

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Merchant and regulated storage investment in energy and reserve markets: a Stackelberg game

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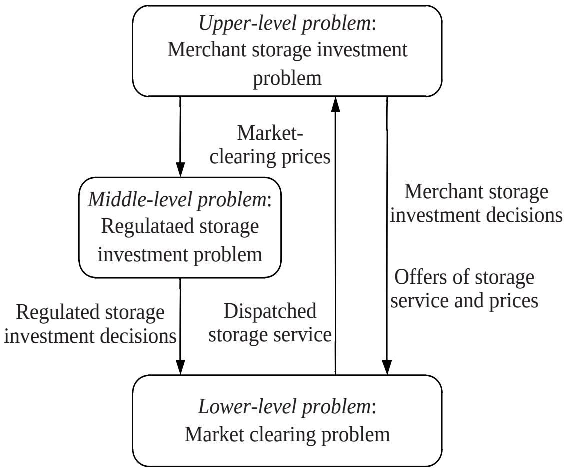
With large-scale integration of renewable generation, energy storage (ES) is expected to play important role in providing flexibility to energy systems. ES can be owned and operated by both system operator (SO) and a private merchant [1]. The ownership structures of ES influence operation strategies and potential benefits realized by the whole energy system [2]. Hence, the studies of ES investment problem roughly fall into two groups: 1) centralized SO investment and 2) profit-maximizing merchant investment. Also, as a flexible resource, ES can perform spatio-temporal energy arbitrage to mitigate the effects of variability and uncertainty coming from renewable energy sources. Furthermore, ES can provide reserve ancillary service to enhance grid's reliability and security.



In this paper, we construct a trilevel Stackelberg game model to study the co-investment of merchant and regulated storage in energy and reserve markets. The trilevel structure of the proposed problem is shown in Fig. 1. The upper-level (UL) problem is a profit-maximizing storage investment problem with a desired rate-of-return solved by a merchant investor. In the middle-level (ML) problem, the SO makes regulated storage investment decisions to minimize system cost. In the lower-level (LL) problem, SO clears the energy and reserve markets.

This trilevel problem cannot be solved directly. We merge the ML and LL problems as a new LL' problem and then derive the KKT conditions of LL' problem, which are taken as the constraints of UL problem. With Big-M method and strong duality theorem, we can get a single-level solvable mixed integer linear program (MILP). We investigate the proposed model using a 6-bus illustrative example. Fig. 2 shows the energy and reserve revenues and profits of merchant storage in three capital cost scenarios. Profit is the difference between storage revenue and investment cost.

The proposed model captures the interactions of regulated and merchant storage investment. Also, it provides an insight for the ownership structures of ES, social welfare, and profitability of merchant storage in the joint energy and reserve market in different desirable rate-of-return, capital cost of storage investment scenarios.

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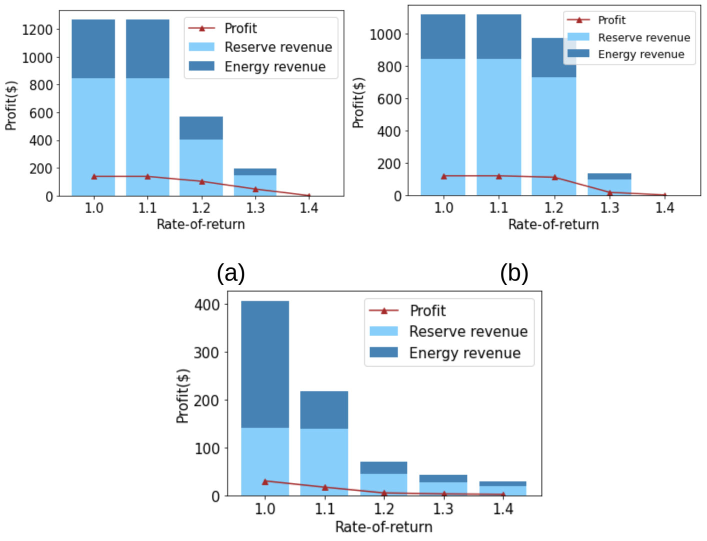

(a)

(b)

(c)

Figure 2: Revenues and profits of merchant storage in three capital cost of investment scenarios: (a) Low, (b) Medium, (c) High.

Laser material processing for the production of fuel cell components

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Polymer electrolyte membrane fuel cells (PEMFCs) are a promising technology for powering a wide range of applications by converting chemically stored energy into electrical energy. However, the relatively high material and production costs and the insufficient durability still limit a commercial usage. Laser material processing can contribute to reduce production costs and increase the lifetime as well as the performance due to its high level of flexibility, productivity, and wear free operation.

Micro structuring of fuel cell diffusion layers

In a PEMFC, hydrogen and oxygen react to water ($2H_2 + O_2 \rightarrow 2H_2O$). The water must be dissipated from the fuel cell by passing through the microporous layer (MPL) and the gas diffusion layer (GDL) to the bipolar plate (BPP). The in-cell water management is decisive for the performance and the lifetime of PEMFCs. The structural modification of the MPL and GDL has already shown promising improvements of the water management in literature [1]. To introduce microdrillings into the different layers, laser systems generating pulses with femto- and picosecond pulse durations can be used as a precise material removal with a low thermal impact into the workpiece is possible.

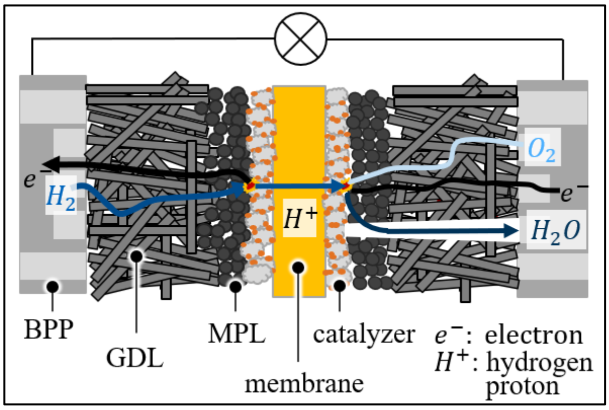

Figure 1: Schematic illustration of a PEMFC with perforated diffusion layers

Inline quality assurance for the welding of bipolar plates

In terms of manufacturing, a variety of materials are being considered for the fabrication of BPP as a core component of PEMFCs. The application of coated stainless-steel foils (e.g., AISI 316L) is favored over other materials, as they show numerous advantages, such as a high thermal and electrical conductivity. Depending on the exact material and the thickness of the metal foils (approx. 50 – 150 µm [2]), observable process instabilities, such as the humping effect, can occur at different welding speeds, reducing the weld seam quality significantly. To monitor the gas-tight joining of two metal foils, different sensor approaches are combined with artificial intelligence to predict the weld seam quality inline.

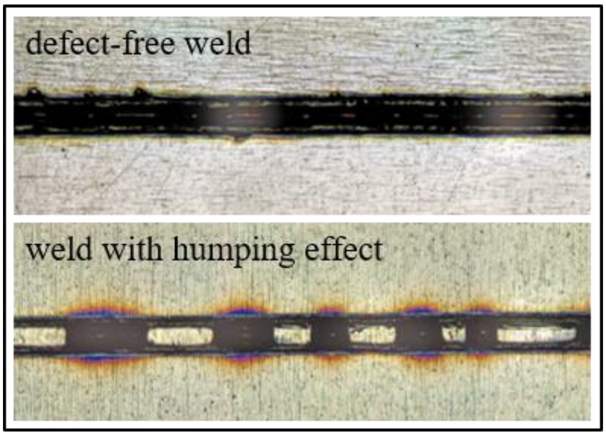

Figure 2: Comparison of a defect-free weld and a weld with the humping effect

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CuTi-based alloys for lightweight constructions in aero- and astronautics

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Bulk metallic glasses (BMGs) based on CuTi feature exciting properties e.g., high strength, large elastic limit, good resistance against corrosion, and biocompatibility, which renders them promising as lightweight alloys in the field of aero- and astronautics.[1,2] These custom-designed alloys have the potential to reduce the overall weight of airplanes and spaceships/satellites, which reduces the amount of fuel and emissions.

In recent years, several multicomponent CuTi-based BMGs with excellent glass-forming abilities (GFA) have been discovered, however the relevant mechanisms on the atomic scale are still to be explored. While multicomponent alloys exhibit the best GFA, the less complex binary CuTi systems is suited for analyzing the glass formation on an atomic level upon solidification from the liquid metal melt. For a fundamental understanding of the glass formation processes, regarding the atomic structures and short-range orders in the undercooled melt, binary CuTi serves as a less complex reference system. We studied composition-dependent packing fraction and short-range order in the binary CuTi liquids in the range of 33 to 76 at% Cu by neutron and x-ray diffraction. Due to the high chemical reactivity of Ti-based melts, the CuTi samples have been containerlessly processed using electrostatic levitation. This technique enables access to the metastable regime of an undercooled melt. In addition, the absence of any container or crucible results in an excellent signal-to-noise ratio in scattering experiments. Figure 1 shows the levitation setup at the P21.1 beamline at DESY, Hamburg (left) and at the D20 beamline at ILL, Grenoble (right).

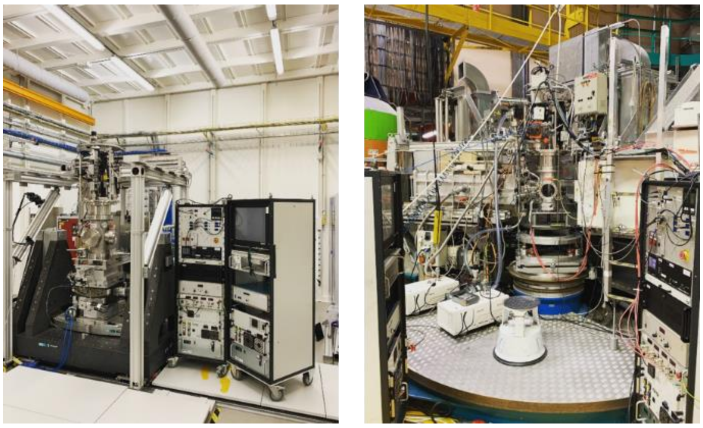

Figure 1: Setup for electrostatic levitation at DESY, Hamburg (left) and ILL, Grenoble (right).

To take full advantage of the different scattering contrasts of the CuTi system, data from neutron scattering and diffraction with synchrotron radiation are combined, which gives information on topological and chemical short-range orders. By correlating structural information with the dynamics of the CuTi liquid, the relationship between structure and dynamics is revealed, which contributes to the development of a fundamental understanding of the glass formation processes on the atomic scale. The achieved knowledge serves as basis for the development of custom-tailored CuTi alloys that combine high strength, high elasticity, and a low weight, and therefore can contribute to a more efficient air- and spaceflights.

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Picosecond Charge-Transfer-State Dynamics in PTQ-2F:BTP-4F-Blend Films Investigated by Time-Resolved IR Spectroscopy

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Organic semiconductors can be used in a wide range of applications. A particular prominent one can be found in the field of solution-processed bulk-heterojunction (BHJ) organic solar cells (OSC), which offer high possible conversion efficiencies.

After photoexcitation, an exciton diffuses towards the donor-acceptor interface where a charge-transfer-state (CTS) is formed. In the later stages, the separated carriers interact with the materials and form polarons, leading to screening.[1]

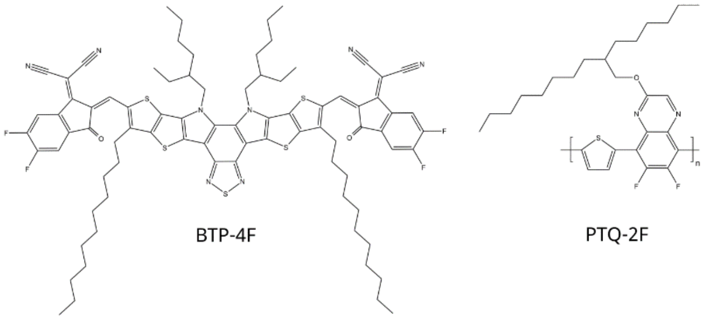

Figure 1: Structural formula of the electron acceptor BTP-4F (left) and the electron acceptor PTQ-2F (right).

To investigate the interaction between polarons and vibrational modes, we employed time-resolved infrared spectroscopy. Here, the occurrence of Infrared Activated Vibrations (IRAV) [2] allows tracking the dynamics of the polaron-structure interaction. In our study, we investigated PTQ-2F:BTP-4F blend films (for the structure formula see Figure 1) coated from different solvents using mIR transient absorption (mIR-TA) spectroscopy, DFT-calculations and GISAXS characterization. We find a series of Fano-antiresonance signals in the mIR-TA spectra together with a broad polaronic background (see Figure 2). Comparing the dynamics of the Fano-antiresonance and the background, an additional process can be observed, independent of whether the electron-donor or –acceptor has been excited. This process, which has a characteristic time on the order of a few to a few tens of ps, is only present in the BHJ samples, but not in the neat acceptor or donor films.

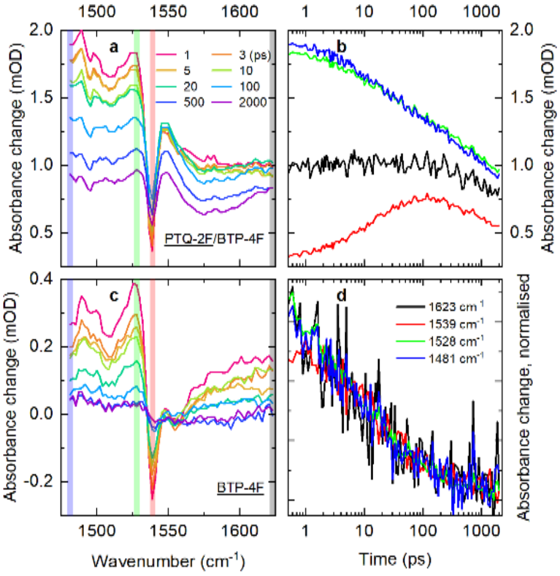

Figure 2: (a) Selected mIR-TA spectra of PTQ-2F:BTP-4F as coated from TMB. (b) Dynamics of the spectral regions highlighted in (a). (c) Seleced mIR-TA spectra of BTP-4F. (d) Normalized dynamics of the spectral regions indicated in(c)

This points to effects associated with the charge-carrier separation, in particular to the CTS. Considering the Fano-interaction involved, we associate the additional early signal with the interaction of electron polarons with the electron donor's vibrational modes in the CTS.

The influence of the structure on the characteristic time has been evaluated with the help of GISAXS measurements. We find a strong influence of the morphology on the CTS lifetime.

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Neutrons to understand improvement in battery performance on electrode modification

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Electric vehicles are on the way to replace gasoline-powered vehicles in our near future. To power such vehicles, Li-ion batteries with very high storage capacities are necessary, so that these cars travel sufficiently large distances before needing a recharge at charging stations. Moreover, these batteries should have long lifetimes so that they can be charged and discharged several times before needing a replacement. Now energy storage capabilities, rate performances and cycling stabilities of Li-ion batteries are strongly dependent on the electrode materials. As practical energy densities accessible with cathode materials are already close to their theoretical limits with the currently available electrolytes, improvements or replacement of anode materials becomes more paramount than the cathode materials. The widely used graphite anode is stable, but offers low energy density, and suffers from side reactions, which are severe at higher charging rates and low temperatures, leading to eventual capacity fading. Titanium oxide anodes offer much longer life cycles, but have even lower energy densities. Li metal anodes offer the highest possible energy density, but are prone to dendrite formation and thus not preferred for safety reasons. Si anodes offer second highest possible energy densities, but suffer from large volume changes leading to fast capacity fading. With help of several analytical methods, including neutron based methods; this contribution will show how battery performances can be enhanced by either altering the anode morphology, or preparing composite anode mixtures, or by applying coatings to anode surfaces.

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Open-mastr Python package

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The Marktstammdatenregister (MaStR) is a German register provided by the German Federal Network Agency (Bundesnetzagentur, short: BNetzA) that keeps track of all power and gas units located in Germany.

The MaStR open data set can be browsed online on the website of the BNetzA, taken from daily provided dumps or be accessed via the web service. The python package open-mastr[1] focuses on the second and the third option. It provides a python interface for accessing data via the bulk download and the web service API and methods to clean the data. The cleaned data is then written to a database. The open-mastr package hence provides an easy access to the dataset which is especially useful in the community of energy system researchers.

Nevertheless, the data source of MaStR are entries made by unit owners and hence prone to errors. To improve data quality, grid operators are required to verify entries over time (See fig. 1). In the future we will develop methods to measure the data quality and increase it.

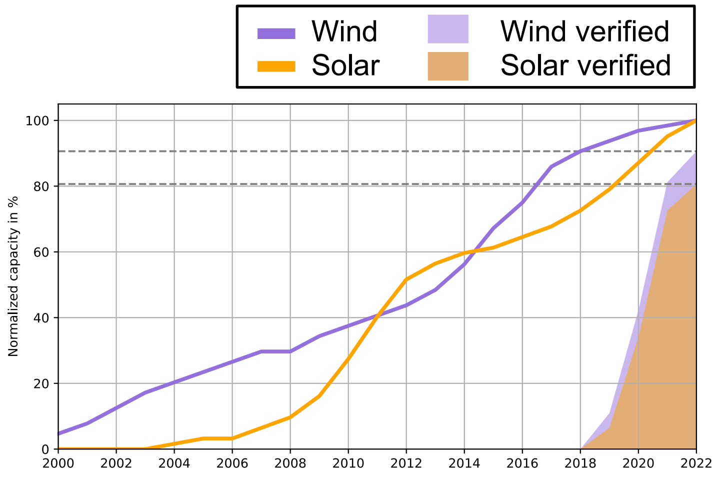

Figure 1 - Wind and solar capacity expansion in Germany

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Image segmentation of photovoltaic systems in Munich

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Due to their relatively small cost, photovoltaic (PV) systems offer participation in the “Energiewende” for millions of house owners in Germany. The size and location of this large number of installed PV systems are included in the Marktstammdatenregister from the Bundesnetzagentur, but this data is erroneous, and the access is restricted. However, knowing the current number, capacity, and location of installations is important for energy system modeling, grid operation, and policymakers.

We aim to extract relevant information about PV systems from a data set of flight images by using computer vision techniques. The data set contains up-to-date images of Munich from recent overflights. Besides creating and optimizing Neural Networks dedicated to the task of object identification, we will also evaluate semi-supervised methods to decrease the manual labeling effort of PV systems for humans.

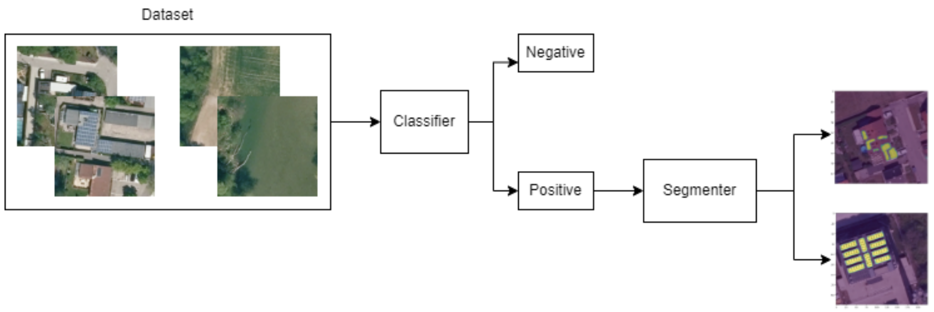

Figure 1: Schematic of supervised image calssification and segmentation model

In our work, we explore different supervision techniques for deep learning-based image segmentation of photovoltaic systems in Munich. As our first approach, PV systems on 7% of available images are manually annotated and used as a dataset for our supervised learning model. The dataset is passed through a classifier first, and only positive samples (images including PV systems) from the classifier are passed to segmentation, where it predicts the PV masks. Output from both classification and segmentation are evaluated using the test set, where the classifier achieves 99% accuracy and segmenter achieves a dice coefficient of >94%.

Due to the challenging and expensive task of annotating the images, we plan on doing semi-supervised learning as our second approach. We train the model on labeled and unlabeled examples since we have many unlabeled examples compared to a few labeled ones. We will use an open dataset from the USA [1] alongside the unlabeled Bavarian images in training the model and making predictions on the Bavarian images. The goal is to have a network that can identify PV systems with high accuracy without needing any additional annotated images.

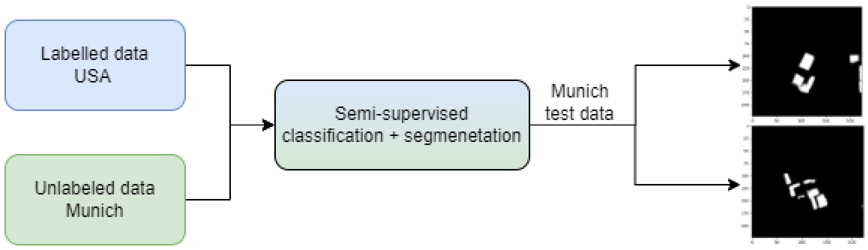

Figure 2: Schematic of semi-supevised learning using data from USA and Munich

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