

Energy Sciences for Europe's Green Deal

11th Colloquium of the Munich School of Engineering
July 28 - 29, 2021



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The Bavarian Prime Minister Dr. Markus Söder unmistakably emphasized the great importance of climate protection in his government declaration on 21st of July 2021, which made it clear that current efforts must be accelerated significantly. The Prime Minister highlighted issues such as the significant expansion of deep geothermal energy in Bavaria. This is of particular importance to MSE, since it is responsible for coordinating the Geothermal Alliance Bavaria (GAB). A research project whose main focus is research in deep geothermal energy.

Climate protection, energy and energy research need to become the central research questions in the next few years and every single university or research institution must, if possible, reposition itself and align its research accordingly.

Today, more is required than just the gradual shift of a few funding mechanisms, but rather a reassessment of the entire research landscape must take place. Energy and climate must be taken into account in all areas of a university: research, teaching and operation of assets and infrastructure. Also all other fields need to understand their relation to the energy field.

The expansion and restructuring of the energy system has to happen rather fast with having a transformation time limited to a few years. Like this, the campus in Garching could become a wonderful living laboratory a benchmark for planning, renovation and operation. If the conversion of such a complex site succeeds in record time, then the conversion of simpler systems would also succeed.

This requires the steady willingness of the university, the state of Bavaria and all other involved stakeholders to act now. No doubt, the problem of climate change is well understood by now but the will to act accordingly is still more fuzzy and less committed. For every prestigious university it is more than timely to go ahead and show that the university as a whole can act in accordance with the needs for sustainability and climate protection, especially related to the energy consumption. The transformation of the campus in Garching to a carbon neutral campus within the next five to ten years would be the right signal of the university that TUM and the state of Bavaria is willing to accept this challenge and to be a frontrunner in clean technology development and education.

Thomas Hamacher
Director Munich School of Engineering

Munich School of Engineering (MSE)

The **Munich School of Engineering (MSE)** of the Technische Universität München is an open platform for all researchers and students at TUM to combine knowledge and visions for the energy systems of tomorrow. The MSE bundles competencies from TUM's faculties to develop comprehensive research programs tackling as well fundamental as applied questions in the areas of energy production, distribution and storage. To ready upcoming generations of engineers and scientists to respond to the challenges of tomorrow, programs on undergraduate, graduate and postgraduate (PhD) level have been developed and are continuously refined. Exceptionally talented students are equipped with a fundamental scientific tool box and an interdisciplinary mindset to become the future leaders in energy research.

TUM.Energy is a cross-departmental research initiative within the MSE, which offers a platform for the so-called "Green Technologies", in particular energy research in the segments Electromobility, Power Plant Technologies, Renewable Energies, and Energy Efficiency. These main topics are represented in networks in which researchers of different departments are working in detail on the challenges within these fields:

- The network **TUM.Battery** supports research on battery technologies. At the Technical University of Munich, more than 100 persons work in this field. Manifold individual projects are carried out in the area of the chairs' and institutes' core competencies, for instance in cooperation with partners from industry, economy, politics and research.
- The network **TUM.<nXfc[Yb/ PtX** coordinates interdisciplinary research on electricity-based future energy solutions, such as hydrogen or synthetic fuels. The goal is to understand systems in their complete value chain - from fundamentals to marketing.
- The **Network for Renewable Energy** is doing research in both, fundamental research in the field of new technologies and materials as well as improvements of existing technologies increasing their applicability.
- **9byf[nl: ccXIK UMF!BYI i g** at MSE explores the connected challenges of energy, food and water in times of urbanization, population rise and climate change. It unites competences ranging from sustainable buildings to vertical farming.
- The **Center for Sustainable Building** is dedicating itself to energy efficiency during the use of buildings and its consideration during planning. Thereby not only technical but also socio-ecologic aspects are integrated in urban planning approaches.
- The **Center for Combined Smart Energy Systems** focuses on modeling the interdependency of electricity distribution, heat, and communication networks and thus sector-coupling. The goal is to develop strategies for integrating extensive distributed energy sources into smart micro grids.

11th Energy Colloquium of the Munich School of Engineering 2nd Virtual Edition

Energy Sciences for Europe's Green Deal

Please register by July 23rd, 2021 to get your login information: <http://www.mse.tum.de>

July 28, 12:30 to 5:30 pm

12:30 pm Opening

Prof. Dr. Thomas Hamacher
Director, Munich School of Engineering, TUM

12:45 pm Keynote

Technologies Enabling the H₂ Value Chain

Dr. Andreas Peschel, Head of Chemical Technology R&D, Linde GmbH,
Linde Engineering

1:15 pm *Fundamentals in Functional Materials*

Session Chair: Prof. Dr. Peter Müller-Buschbaum

Comparison of the Temperature-Dependent Impedance and Rate Performance of Silicon and Graphite Anodes

Clara Berg, Chair of Technical Electrochemistry, TUM

Top-Down Synthesis of Pt-Based Oxygen Electro-Reduction Catalysts

Dr. Batyr Garlyyev, Department of Physics, TUM

A Concept of a μ -Photoreactor for Planar Hydrogen Evolution Catalysts at Ambient Conditions

Clara Aletsee, Chair of Physical Chemistry, TUM

2:30 pm Coffee Break

2:45 pm *Innovative Technologies and Applications*

Session Chair: Prof. Dr. Andreas Jossen

Emerging Thin-Film Solar Cell Technologies Reaching Space

Lennart Reb, Department of Physics, TUM

Water-Based Prussian Blue Ink Optimization by Using High-Throughput Robotic System for Electrochromic Smart Windows

Oleksandr Mashkov, i-Meet, FAU

Development of Innovative Nano-CHP Using New Thermoelectric Generators (TEG)

Arne Stumpf, Competence Center Thermal Energy Systems, TH Nuernberg

4:00 pm Keynote

Energy Demand in the Built Environment - Strategies for Sector Coupling

Kerstin Vogt, VdZ

4:30 pm Poster Session I

Join us for a virtual get together!

July 29, 9:00 am to 5:30 pm

9:00 am Workshop - Energy Scenarios for Bavaria

The STROM-Project investigates the future of the energy system in Bavaria with a special focus on heating sector and the interaction between heating and power sector. The development will depend pretty much on the development of the Global, European and National energy system. Therefore the workshop will define the possible scenario frames we need to consider and will also discuss the central technologies which most likely will be of prime importance for the project. An example which will be highlighted in the workshop is deep geothermal energy for heat production.

12:30 pm Poster Session II

1:30 pm Opening

Prof. Dr. Thomas Hamacher

1:45 pm Keynote

Security of Supply – Concept of Evaluation

Dr. Philipp Kuhn, Chair of Sustainable and Renewable Energy Systems, TUM

2:15 pm *Innovative & Improved Energy Conversion Technologies*

Session Chair: Prof. Dr. Hartmut Spliethoff

BioCORE- Highly Efficient Biogas Conversion in Reversible Solid Oxide Cells

Felix Fischer, Chair for Energy Systems, TUM

Utilization of Wood Gas in a SOFC-Stack

Federica Torrigino, Chair of Energy Process Engineering, FAU

Compact and Cost-Efficient Cold Storage Based on an Absorption Process with H₂O/LiBr

Dieter Pressl, ZAE Bayern

3:30 pm Coffee Break

3:45 pm *Impacts on Energy Supply in the Near Future*

Session Chair: Prof. Dr. Thomas Hamacher

Battery-Assistance vs. Grid Reinforcement for High-Power EV Charging: An Emissions Perspective

Anupam Parlikar, Institute for Electrical Energy Storage Technology, TUM

Can the Environmental Impact of Wind Turbines be Reduced through Design?

Helena Canet, Chair for Wind Energy, TUM

Environmental Effects of Digitization for Smart Grid Use Cases – a Life-Cycle Perspective and Beyond

Daniela Wohlschläger, Forschungsstelle für Energiewirtschaft

5:00 pm Keynote

What Factors Influencing the Adoption of Green Hydrogen: A Global Perspective

Prof. Dr. Svetlana Ikonnikova, Center for Energy Markets, TUM

5:30 pm Summary and Closing

Prof. Dr. Thomas Hamacher

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1. Oral Presentations

Comparison of the Temperature-Dependent Impedance and Rate Performance of Silicon and Graphite Anodes

Clara Berg^a, Robert Morasch^b, Maximilian Graf^c, Hubert A. Gasteiger^d

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Silicon is a promising candidate for replacing graphite in anodes for lithium-ion batteries due to its high theoretical capacity and its encouraging rate performance. However, it suffers from large volumetric changes upon (de-)lithiation which significantly compromise the cycling stability.^[2] Jantke et al.^[1] reported the reversible cycling of an affordable microsilicon material. By utilizing a third of the full theoretical capacity of silicon and thus limiting the volumetric expansion, the microparticles can withstand the mechanical strain without particle pulverisation and degradation. Electrodes with 70%_{wt} of microsilicon are only approximately 40% of the mass of a graphite electrode with the same capacity. This difference in electrode mass loading has implications on the electrodes' kinetic properties.

In this study, the temperature-dependent impedance and rate performance of silicon and graphite electrodes with matched capacities - and therefore different mass loadings - are compared (Fig. 1). Different relative contributions of the ionic pore and charge-transfer resistances are identified by an impedance analysis. As the path of an ion through the thin silicon electrode is short there is only a small contribution of ionic pore resistance. At the same time, the lower mass loading compared to that of the graphite electrode implies a smaller absolute active material surface area resulting in higher charge-transfer resistance. As the activation energies for ionic conductivity and charge-transfer differ significantly, silicon and graphite electrode kinetics exhibit different temperature dependencies. In this study, these dependencies are related to the rate performance at different temperatures.

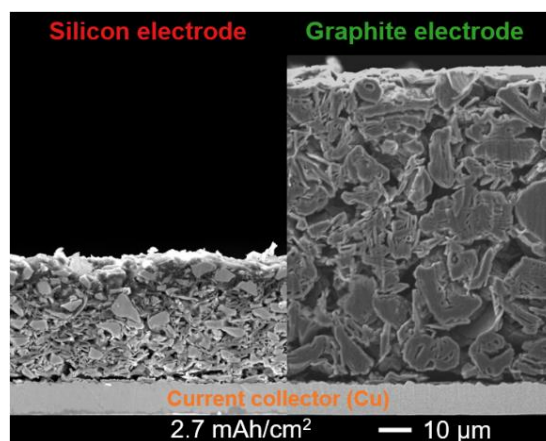


Figure 2: Scanning electron microscopy (SEM) images showing the cross-sections of pristine silicon and graphite electrodes with a capacity loading of 2.7 mAh/cm² calculated by referring to the reversible capacities of 1200 mAh/g_{Si} and 350 mAh/g_{Gra} for the silicon and graphite electrodes respectively. SEM specifications: secondary electron detection, 10.0 kV electron acceleration voltage, × 500 magnification.

References

- [1] N. Obrovac, V. L. Chevrier, *Chemical Reviews*. **114**, 11444 (2014).
 [2] Jantke D, Bernhard R, Hanelt E, Buhmester T, Pfeiffer J, Haufe S. *Journal of the Electrochemical Society*. **166**, A3881 (2019).

Top-down synthesis of Pt-based oxygen electro-reduction catalysts

Batyr Garlyyev,^a Johannes Fichtner, Sebastian A. Watzele, Aliaksandr S. Bandarenka

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One of the key factors limiting the widespread applications of fuel cell technologies is the cost of the electrocatalysts utilized in catalyzing the oxygen reduction reaction (ORR) at the cathode side. More specifically, only platinum based electrocatalysts have shown sufficient activity; however, due to the scarcity and cost of Pt, it is of a particular interest to increase their activity per mass. We tackle these challenge by optimizing the size, shape and composition of Pt-based nanoparticles.

Results from Pt model catalyst surfaces have demonstrated that surface defects, in particular surface concavities, can improve the ORR kinetics. It is, however, a challenging task to synthesize nanostructured catalysts with such defective surfaces. Hence, we produced Pt/C catalyst with high density of surface concavities, which was confirmed by high-resolution transmission electron microscopy, 3D-tomography, high energy X-ray measurements and positron annihilation spectroscopy (**Figure 1**). The ORR activity of the developed catalyst exceeds that of commercial Pt/C catalyst, at least 2.7-times in terms of specific ($\sim 1.62 \text{ mA/cm}^2$ at 0.9V) and at least 1.7-times in terms of mass activity ($\sim 712 \text{ mA/mg}_{\text{Pt}}$), which can be correlated to the enhanced amount of surface defects. Furthermore, the alloyed Pt_xPr nanoparticles were synthesized and their ORR activity was investigated. The alloyed nanoparticles showed 4-fold enhancement in the specific activity and 1.5 times increase in mass activity in comparison to the commercial catalyst (**Figure 2**).

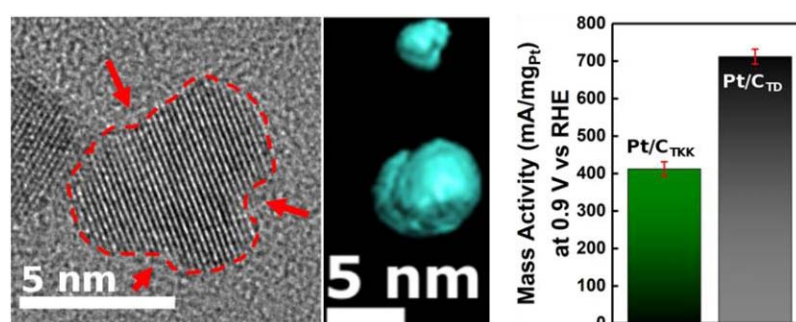


Figure 1. The ORR activity of Pt nanoparticles with high density of surface concavities. High resolution TEM and 3D Tomography images with mass activity of the Pt nanoparticles are shown in comparison to commercial Pt/C catalyst

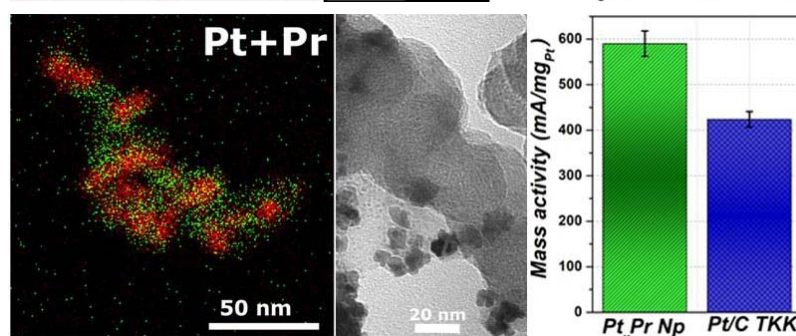


Figure 2. The ORR activity of alloyed PtPr nanoparticles. TEM and EDX mapping images with mass activity of the PtPr nanoparticles are shown in comparison to commercial Pt/C catalyst.

References:

1. Fichtner, S. Watzele, B. Garlyyev, A.S. Bandarenka. ACS Catal. 2020, 10, 3131-3142.
2. B. Garlyyev et al. Nano Research (2020) <https://doi.org/10.1007/s12274-020-3281-z>
3. J. Fichtner, B. Garlyyev, S. Watzele, et al. ACS Appl. Mater. Interfaces, 2019, 11, 5129-5135.

A Concept of a μ -Photoreactor for Planar Hydrogen Evolution Catalysts at Ambient Conditions

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Photocatalytic water splitting and alcohol reforming offer exciting opportunities for the clean H₂ production, in contrast to the industrially applied steam reforming, which requires fossil fuel as a feedstock. Intensive research efforts devoted to these reactions have resulted in a high quantity of structurally complex powdered photocatalysts. However, the processes are not yet industrially realized since the developed catalysts are too inefficient in the visible light range. Furthermore, their complexity makes a mechanistic understanding and hence their systematic improvement towards high performance virtually impossible. Therefore, the preparation of compounds with well-defined atomic level characteristics represents an attractive approach to overcome these issues. Such model substrates are already used for fundamental studies in the ultra-high vacuum (UHV), but a simple extrapolation of the results to applied conditions is impeded by a pressure difference of nine orders of magnitude. The evaluation of ideal photocatalysts under ambient conditions will yield more realistic and exploitable information but is currently not possible due to the lack of suitable test setups.

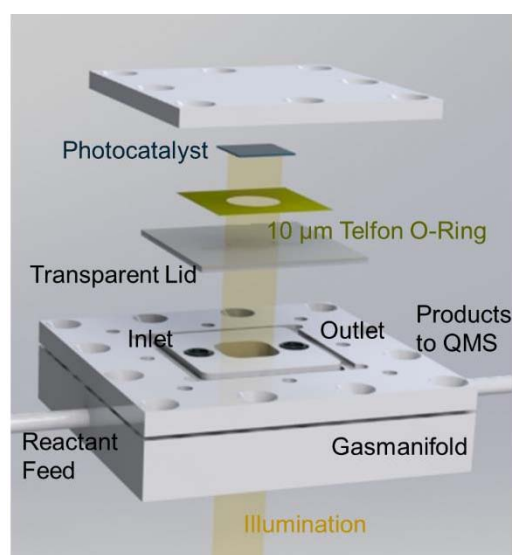


Figure 1: Concept of the μ -Photoreactor.

In the next step, the gas phase μ -photoreactor will be implemented into a flow and pressure controlling infrastructure, allowing the feeding of various reactants such as alcohols, water, or CO₂. Its design enables not only kinetic evaluation of planar photocatalysts by utilizing different lids with defined gas flows but also material characterization after catalysis, unparalleled to date. Thereby, different photocatalysts within the e-conversion project can be investigated under variable, yet comparable conditions. Differences in the reactive behavior with respect to the environment will contribute to a fundamental understanding of reaction pathways. This is vital to ultimately facilitate significant advancements within the rational design of H₂ producing photocatalysts.

In this contribution, we present a novel concept for a μ -photoreactor enabling the evaluation of planar catalysts such as single crystals, nanowires, and other samples developed in the framework of e-conversion at ambient conditions in a continuous gas flow. The planar catalyst serves as the bottom of the reactor, while a 10 μ m teflon O-ring on top defines a reactor volume as low as 640 nL. The system is closed by a UV-vis transparent pyrex (SiO₂) lid with implemented gas flow channels for the reactant flow over the catalyst surface towards the quadrupole mass spectrometer (QMS) for product analysis. The low total gas flow (μ L/min) and small reactor volume guarantee a highly sensitive detection of the products and fast response times. The μ -sized flow channels are incorporated into the lid by photolithography and etching in a multistage process uniting several crucial features for sensitive detection. The total gas flow is defined by a capillary at the outlet, which also accounts for the required pressure drop from reactor chamber to the QMS. At the inlet, a constriction limits the back diffusion of reactants and products. The lid evaluation by profilometry and microscopy allows the prediction of gas flow, back diffusion, and pressure.

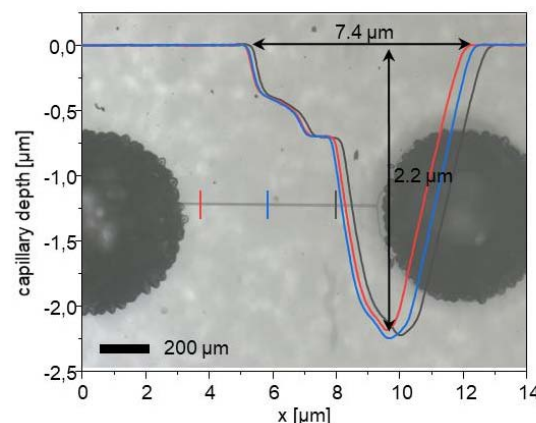


Figure 2: Geometric evaluation of the etched capillary in the SiO₂ lid by microscopy and profilometry for flow prediction.

Emerging Thin-Film Solar Cell Technologies Reaching Space

Lennart K. Reb^a, Michael Böhmer, Benjamin Predeschly, Sebastian Grott, Christian L. Weindl, Goran I. Ivandekic, Renjun Guo, Christoph Dreißigacker, Roman Gernhäuser, Andreas Meyer, Peter Müller-Buschbaum^b

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The emerging technologies of thin-film perovskite and organic solar cells are currently becoming more and more interesting for commercialization. Their steadily increasing record efficiencies from laboratory test cells are approaching those of conventional silicon solar cells, and it is only a matter of time until perovskite solar cells will surpass silicon solar cells in terms of efficiency. These results for solar cells that are solution-processable at ambient conditions open up novel ways for solar cell manufacturing, such as sprayed or printed solar cells on thin flexible plastic foils, i.e. for high throughput techniques on an industrial scale. Besides the terrestrial applications, space exploration will also benefit from lightweight and flexible space panels.

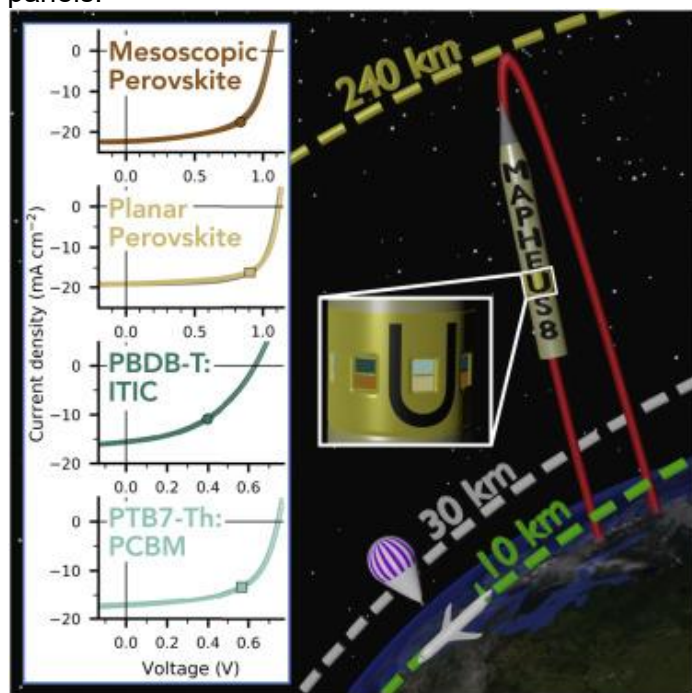


Figure 1: Graphical abstract giving an overview of the solar cell rocket experiment. [1]

In the last years, the research community began to investigate more and more the stability of these systems in different environmental conditions to identify and prevent degradation pathways and thereby increase their lifetime. 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.

Here we present the very first electrical characterization of emerging perovskite and organic solar cells under space conditions at orbital altitudes [1]. During a suborbital rocket flight, we measured the power of our solar cells under different illumination conditions. Our results show that the solar cells survived the harsh conditions during the rocket launch, generated promising amounts of power during strong solar illumination that are comparable with laboratory measurements, and also produced energy in faint light conditions with only indirect solar illumination.

These results show the versatility of perovskite and organic solar cells for application in various environmental conditions, with promising potential to revolutionize not only space exploration.

[1] L. Reb et al., Joule 4, 1880–1892 (2020).

Water-based Prussian blue ink optimization by using high-throughput robotic system for electrochromic smart windows

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Electrochromic materials are a type of chromic compounds capable of reversibly changing their color or opacity under external applied potential. The installation of facade panels equipped with electrochromic materials offers temporary control of the transmitted solar energy and seems to be one of the solutions to reduce the use of air conditioning systems inside buildings and thus energy consumption. Prussian blue, $\text{Fe}^{\text{III}}_4[\text{Fe}^{\text{II}}(\text{CN})_6]_3$, is not only a blue pigment widely used in art, but also a beautiful representative of electrochromic materials, non-toxic and low-cost in preparation (in comparison to other electrochromic compounds: ReO_3 , WO_3 , ITO, Nb_2O_5 , VO_x etc), and able to change its color from blue to colorless. The widespread method for the synthesis of Prussian blue involves high energy-consuming electrochemical deposition from solutions of the corresponding salts ($\text{K}_3[\text{Fe}(\text{CN})_6]$ and FeCl_3). Here we developed a suitable

composition of an aqueous ink based on colloidal synthesis of Prussian blue nanocrystals for the fabrication of thin electrochromic films. By using a high-throughput robotic setup we achieved the optimal ratio of components (Prussian Blue NCs – 75 mg/mL, Zonyl – 6 wt.%, and DMSO – 7.5 wt.%) in the ink to achieve the maximum optical density of the film with the minimum possible number of deposited layers. To demonstrate the electrochromic properties of the Prussian blue film, a "smart window" consisting of three components (an electrochromic material, a polymer organic electrolyte, and an ionic storage layer) was made. The storage layer in this work is a film of colloidal CeO_2 nanocrystals in which the fatty ligands have been removed using EDT cross-linking ligands. Application of the potential modulates the

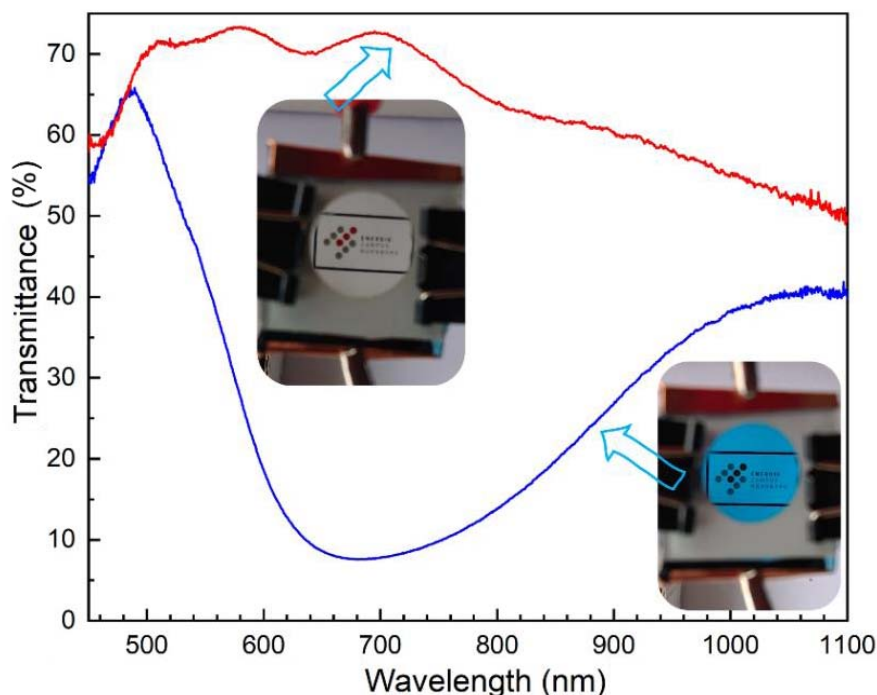


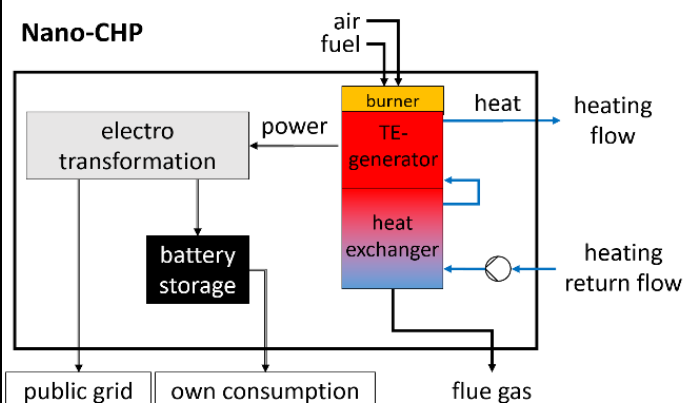
Figure 1: Transmittance of electrochromic device based on Prussian Blue NCS and CeO_2 NCS.

transmittance of the device at 680 nm from 7.6% to 72.2%. The facile preparation of electrochromic ink, as well as the low-temperature post-deposition annealing, is promising for industrial applications of electrochromic foils, whose fabrication can easily be upscaled by roll-to-roll printing technologies.

Development of innovative Nano-CHP using new thermoelectric generators (TEG)

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Our project's goal is to develop a combined heat and power unit (CHP) for converting waste heat from heating in single-family houses into electrical energy. Several industrial and research partners are engaged in our project which is a ZIM-project funded by the BMWi.

In contrast to conventional CHP concepts, which use conventional combustion engines, our concept uses thermoelectric modules (TEMs) to generate electricity and a commercial condensing boiler to generate thermal energy. We use Skutterudite and bismuth telluride semiconductors as a basis for the high-temperature TEMs. The temperature gradient between hot flue gas and cooling water is the driving force and responsible for generating electrical energy.

Figure 1: Schematic concept of Nano-CHP with TE-generator

The thermoelectric generator (TEG) comprises approx. 20 TEMs, which are connected electrically in series-parallel and thermally in parallel. The new nano-CHP will generate electricity with minimal CO₂ emissions, thus offering the private sector the opportunity easily to reduce its CO₂ footprint. The TEG is inexpensive and can be implemented easily. The great advantage of the new technology is the use of a commercially available, highly efficient condensing boiler. This enables demand-based power generation for private households with highly efficient heat generation, high flexibility, and short response times. This is a major difference to the available CHP systems for household applications.

One of the greatest challenges of the project is to supply the TEMs with the ideal amount of heat at each operating point. The ideal amount of heat ensures that the TEG performs well and thus generates a significant amount of electricity. To solve this challenge, it is essential to control precisely the heat flow from the hot flue gas to the TEG and from the TEG to the heating water. The hot gas temperature is around 1000 °C and the material temperatures are at around 550 °C. This poses challenges for the mechanical construction of the TEG, which finally must be also economically feasible.

The presentation gives an overview of the ongoing ZIM-project and shows some current results. The main topics of the presentation are the current results of the simulation of the hot gas heat exchanger such as temperature and flow profile, as well as the pressure loss. The presentation explains the idea and concept of nano-CHP with TEMs, the used models in the simulation, and why this concept is superior to conventional CHP concepts.

In addition, the experimental results are discussed and compared with results from simulation and previous works. Finally, the profitability of a private, domestic nano-CHP using TEMs, is assessed and compared to some conventional CHP concepts such as internal combustion engines and fuel cells.



Figure 2: Condensing boiler with TEG

BioCORE – Highly Efficient Biogas Utilization in Solid Oxide Fuel Cells

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The energy system of the future will be largely based on renewable energies (especially wind/PV). However, their fluctuating electricity production requires additional measures to balance supply and demand. Biogas is one of the few renewable energy sources that can provide both secure base load and balancing power. At present, however, this resource is usually converted in combined heat and power plants (CHP) at constant output with electrical efficiencies of less than 40% in about 9,500 plants in Germany alone, or about 18,500 Europe-wide, respectively.

In contrast to the traditional CHP approach, the highly innovative BioCORE technology converts valuable biogas into electricity twice as efficiently, with the additional option of converting the CO₂ (up to 50% of the biogas volume) into synthetic natural gas. High-temperature Solid Oxide Cells are used, which can be operated as fuel cell (SOFC) and as electrolysis (H₂O and CO₂ electrolysis, hydrogen or biomethane production, SOEC) and thus make a considerable contribution to stabilizing the energy system. By using the existing natural gas infrastructure, besides flexibilizing electricity from biogas, the BioCORE technology also solves the problem of long-term storage.

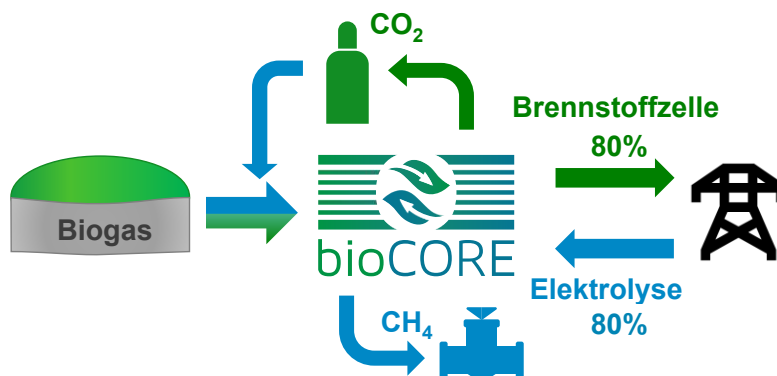


Figure 1: Schematic flowsheet of the BioCORE process – Fuel Cell mode in green, Electrolysis operation in blue

The presentation will provide insights and latest results from the operation of the 10 kW demonstrator that has been put into operation at the Chair of Energy Systems late 2020.

Utilization of wood gas in a SOFC-stack

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Fuel cells represent an environmentally friendly alternative to fossil fuels in the field of energy production. In particular, high-temperature fuel cells (*solid oxide fuel cell*, SOFC) are considered a valid option for cogeneration applications compared to other fuel cell technologies, due to their fuel flexibility, high efficiency, and high-quality waste. Since a single SOFC has a relatively low power density, (approx. 1 W/cm²), multiple single cells are joined together in series to form a stack for technical applications. [1]. However, in order to make a SOFC an interesting option for commercialization, some issues still need to be solved. Besides economic feasibility, the most challenging hurdle is achieving degradation-free SOFC operation over a long time. In fact, during standard SOFC operation, various degradation mechanisms causing performance losses can occur. Electrochemical impedance spectroscopy (EIS) is considered to be one of the most promising methods to characterize these losses.

At the chair of Energy Process Engineering at the Friedrich Alexander University (FAU) of Erlangen-Nuremberg in close cooperation with the company NOVUM Engineering GmbH the coupling of wood-gasification with a commercially available SOFC-stack (Galileo 1000 N, Hexis AG) was realized and the effect of the fluctuating gas quality was investigated by means of EIS. In the case of fluctuating gas quality or unfavorable operating conditions, degradation effects (e.g.: nickel oxidation at the anode) can often be observed within the cell [2,3]. Using impedance measurements (EIS in-situ investigation, frequency range 0.13 Hz-10 kHz, excitation currents 100-140 mA), it is possible to perform online diagnostics to detect critical operating conditions and degradation processes. Each physical process in a SOFC is characterized by a time constant τ , known as relaxation time, which contains information about the speed at which a process occurs. An analysis of the distribution of relaxation times (DRT) enables an accurate interpretation of the EIS results and the identification of the different processes occurring in a SOFC. In Figure 1 a DRT-plot in syngas and real wood gas operation (different H/C ratios) of the stack at 820°C is shown. With the aid of the EIS results, the stack operating conditions can thus be optimally adjusted to prevent possible degradation phenomena. The results presented focus firstly on a variation of the operating temperature and volume in continuous operation with commercial natural gas and pure hydrogen ($\geq 99.9\%$ purity). In addition, different fuel compositions with synthetic syngas (H₂, CO, CO₂, N₂) and real wood gas produced from a laboratory gasifier have been analyzed.

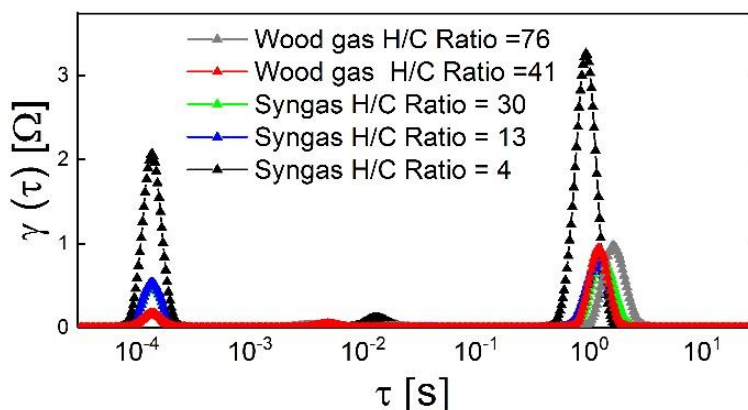


Figure 1: DRT-plot in syngas and real wood gas operation at 820°C.

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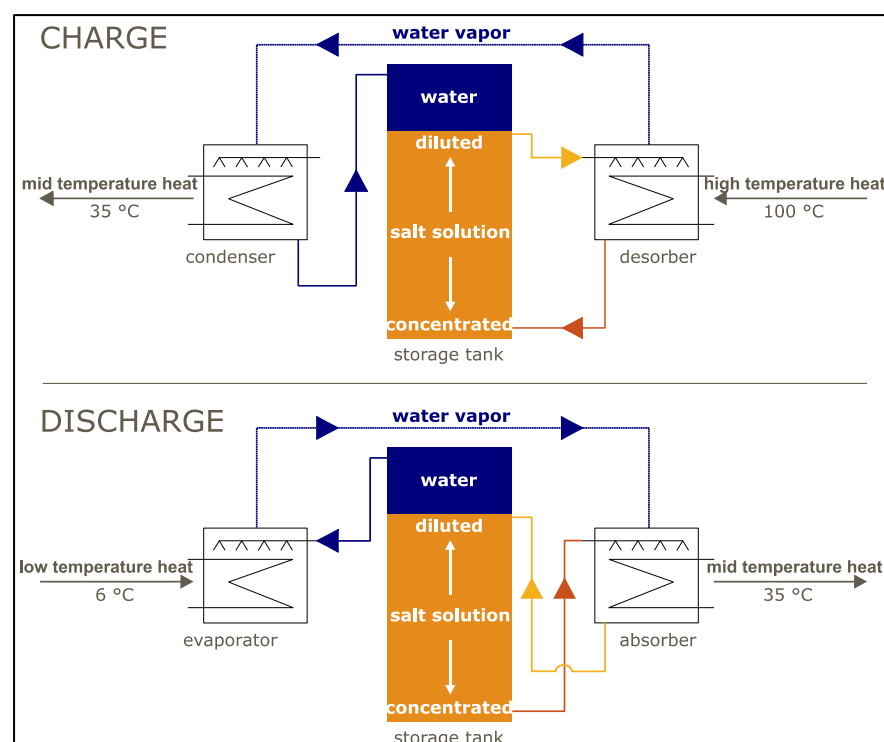
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Compact and cost-efficient cold storage based on an absorption process with H₂O/LiBr

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In the industrial sector, absorption chillers can be a sustainable technology for cold supply if waste heat is used as driving heat source. However, its use often is impeded by a temporal mismatch between availability of waste heat and cooling demand. An approach to overcome this hindrance is the realization of a thermal



absorption storage process, which is a flexible absorption chiller process with integrated energy storage. The fundamental process is depicted schematically in fig. 1. In charging mode, high temperature heat at about 100 °C is used to desorb water vapor from a diluted salt solution, which thereby gets concentrated. The heat of condensation is released to the ambient. The concentrated salt solution is transferred to a storage tank and stores the former thermal energy in the form of free energy. In discharging mode, low temperature heat is extracted from a heat transfer fluid, which thereby is chilled, and is used to evaporate water. The water vapor is absorbed by concentrated salt solution from the storage tank. The mid temperature absorption heat is released to the environment.

Figure 1: Scheme of the absorption cold storage process

The achievable energy density of the storage process fundamentally depends on the difference in salt mass fraction between the concentrated and diluted salt solution. In absorption chillers, it usually does not exceed 3-4 m%, which means that no significant storage effect can be achieved. One of the main goals in the design of a thermal absorption storage process therefore is the maximization of the difference in salt mass fraction. Hence, the salt mass fraction of the diluted salt solution has to be minimized, while the salt mass fraction of the concentrated salt solution has to be maximized.

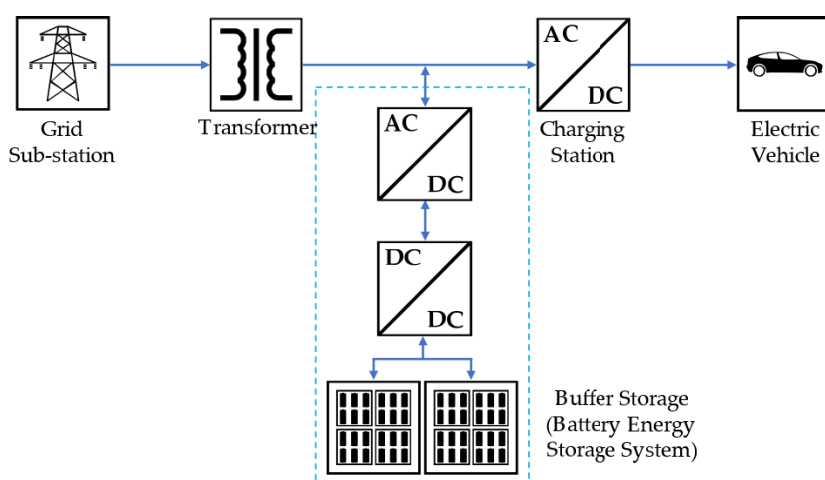
The objective of the presented work was to develop a novel process design of a thermal absorption storage based on H₂O/LiBr with high energy density. This enables a both compact and cost-efficient cold storage. The salt mass fraction of the diluted salt solution is minimized by reducing significantly the specific salt solution mass flow at the absorber. Additionally, the salt mass fraction of the concentrated salt solution is maximized by the formation of LiBr-monohydrate accepting partial crystallization of the solution. The theoretical energy density of the resulting process amounts up to 350 kWh/m³ and therefore significantly outnumbers currently used ice storages. A first economic evaluation of the process resulted in specific storage costs of about 30 €/kWh.

Battery-Assistance vs. Grid Reinforcement for High-Power EV Charging: An Emissions Perspective

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An increasingly large number of battery electric vehicles (BEVs) and electric buses are hitting the roads globally each year. These numbers are expected to grow further in light of ever-more favourable costs, and improved battery technology that addresses concerns about range anxiety and charging times. This upward trend in electrification of the automobile sector essentially shifts the mobility energy demand from the oil & gas sector to the electricity sector. Power transmission bottlenecks in the grid, caused on the supply-side by periods of strong renewable generation, may get further aggravated by adding demand-side bottlenecks to the mix as well. The grid, at several locations, will need to be overhauled to be able to supply huge bursts of power intermittently to cover large power demands to support fast-charging simultaneously at multiple locations. This can entail huge monetary investments for the upgradation of grid infrastructure. Battery-assisted high power charging (BA-HPC) is thought of as a convenient solution to this problem. This solution enables demand-side peak-load shaving, and draws energy more uniformly over extended periods of time. While this solution may well be economically profitable in some cases, an investigation of the environmental impact of this solution can yield interesting insights, and aid decision-makers by identifying scenarios in which one solution is more favorable over the other. This is crucial, since the rationale for shifting to electromobility is the curbing of greenhouse gas emissions. In this work, we employ in-house python-based time-series analysis simulation tools to simulate the grid reinforcement and the battery energy storage systems, and present comparative lifetime emissions analyses for both solutions in a variety of configurations.



Battery-Assisted High-Power Charging

Grid Reinforcement for High-Power Charging

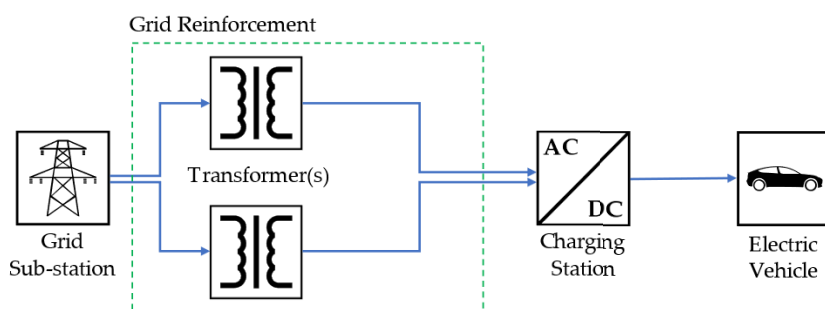


Figure 1: Overview of the two EV charging solutions

Can the environmental impact of wind turbines be reduced through design?

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Wind turbines capture kinetic energy from the wind to produce electricity without directly releasing pollutant emissions. Even though the overall environmental impact of electricity from wind is significantly lower than in the case of fossil-based sources, there is still a significant potential for improvement.

Indeed, multiple processes at different stages of the life-cycle of a wind turbine can have a negative impact on the environment. For example, the extraction of raw materials – such as the rare-earth elements present in the generator – can have a significant environmental impact; similarly, the end-of-life treatment of some components with limited recyclability, such as the blades – generally made of reinforced thermoset polymers – might release polluting emissions into the atmosphere.

With an ever-growing number of wind turbines being manufactured, but also decommissioned, time is ripe to accelerate the efforts to make wind energy even more sustainable. This is a substantial and highly multi-disciplinary challenge, which is already being tackled from different perspectives.

This work proposes to approach this challenge from a design point of view. While modern wind turbines are generally designed for minimum levelized cost of energy, this work proposes to consider the sustainability of the different processes involved in the entire life-cycle of a wind turbine already at the preliminary design stage. The work is organized in two parts.

The first part analyses the environmental impact of modern wind turbines. An impact model is here formulated, which, following a life-cycle assessment (LCA) methodology, quantifies the environmental effects of all the different life-cycle phases of a wind turbine in terms of equivalent greenhouse gas (GHG) emissions. The application of the impact model to an onshore 3.4 MW reference machine unveils the uneven environmental impact of the different components during the turbine life cycle (Figure 1). Indeed, the study identifies the tower as the component with the highest environmental impact, due to its large amount of steel, being responsible for 40% of the overall environmental impact.

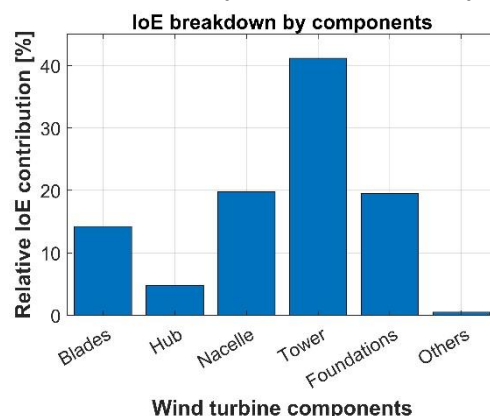


Figure 1. Contribution of each component to the overall environmental impact of a wind turbine.

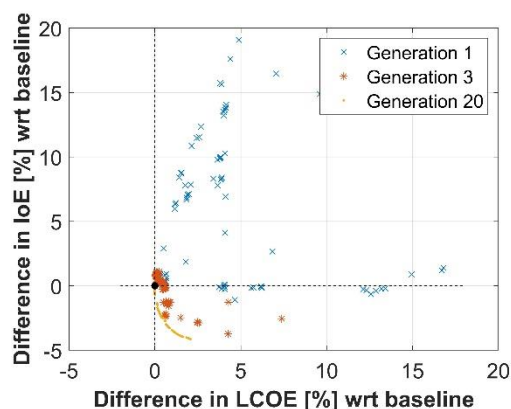


Figure 1. Pareto-optimal front obtained by minimizing levelized cost of energy (LCOE) and environmental impact (IoE). The black dot represents the baseline.

The second part focuses on the formulation of a novel eco-conscious design approach. This approach considers the environmental impact of the wind turbine during its lifetime. The reference turbine is here redesigned based on the new proposed environmentally aware criterion. A family of Pareto-optimal wind turbines is obtained by minimizing the two objectives represented by the overall environmental impact of energy and its levelized cost (Figure 2). This family of solutions trades benefits to the consumer (in terms of a reduced LCOE) with benefits to society (in terms of a reduced environmental impact).

Furthermore, the scope of the design approach is broadened by also considering the impact of the turbine in the grid GHG emissions.

Environmental Effects of Digitization for Smart Grid Use Cases – a Life-Cycle Perspective

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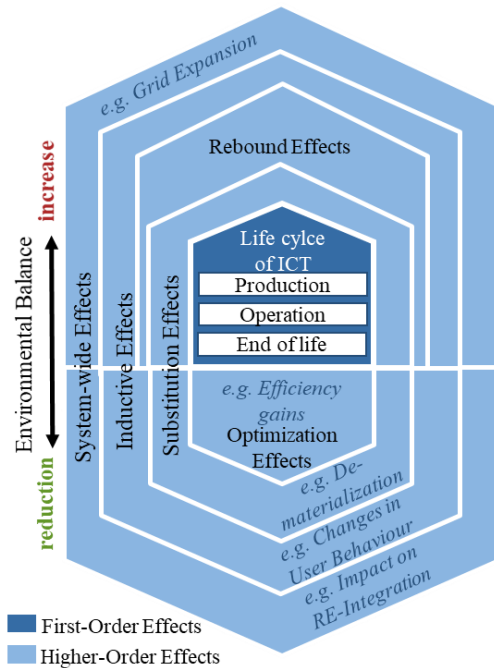


Figure 1: Environmental effects of ICT within smart grids, based on [1], [2]

In combination with the integration of decentralized renewable energies (RE), the progressing electrification of the heating and mobility sector stresses historically established distribution grid structures. Regarding the expansion of electric vehicles (EV), vehicle-to-grid (V2G) concepts can serve as grid stabilization measures for distribution grid operators (DSO). By applying bidirectional charging strategies, EV batteries become flexible storage elements that can both withdraw and feed electricity back to the grid as needed. Thus, the investigated V2G-use case allows the DSO a flexible control of bidirectional EV charging for grid stabilization purposes. Despite the potential contribution to decarbonization, the implementation of required information and communication technology (ICT) and data processing causes a certain expenditure of energy and resources. This includes the establishment and operation of a standardized communication infrastructure between the flexibility asset (e.g. wallbox) and external market participants (e.g. DSO), provided through the rollout of intelligent metering systems (iMSys). As displayed in Fig. 1, environmental effects of ICT-based products or services can be both positive and negative and are distinguished between first-order (direct) and higher-order (indirect) effects [1], [2]. Accordingly, first-order effects consider the energy demand or emissions resulting from a life cycle assessment (LCA) on components. Higher-order effects

concern effects beyond the technology perspective, including rebound effects caused by user behavior, or system-wide effects, e.g. impacts on grid expansion RE integration.

The purpose of this work is to provide a method to quantify direct environmental effects associated with smart grid use cases. The method is applied on the V2G-use case for grid stabilization. Fig. 2 shows the resulting system boundaries of the LCA. The assessment includes components on a household level (wallbox, iMSys, other devices) as well as impacts caused by data processing. Overall, the aim is to determine relevant parameters for a sustainable technical design of digital infrastructure based on empirical results. For a holistic environmental assessment, further investigations on higher-order effects are recommended.

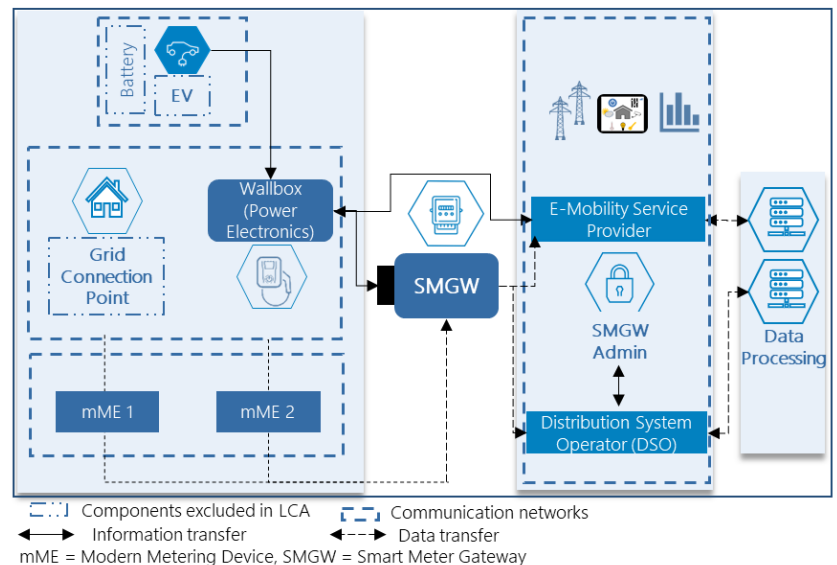


Figure 2: System boundaries for the LCA to assess direct effects of V2G

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2. Posters

Assessment of Active Centers on Transition Metal Surfaces for the Oxygen Reduction and Evolution Reactions

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To economize the resources of our world, research should focus on the use of sustainable technologies such as fuel cells and electrolyzers. However, their potential is limited by the sluggish reaction kinetics of the oxygen reduction (ORR) and evolution (OER) reactions. Suitable electrocatalysts are needed to overcome these issues. Fundamental for smart catalyst design is the knowledge of their active sites. Here, we demonstrate a valuable tool for the in-situ identification of active sites with a resolution down to the nanometer or even atomic scale.

The technique is based on electrochemical scanning tunneling microscopy (EC-STM) which provides potential control to allow (“on”) or inhibit (“off”) a reaction at the sample surface. In the course of a reaction, continuous changes in the composition and structure of the tunneling medium lead to continuous changes in the tunneling barrier. Thus, the STM signal exhibits an increased noise level for reaction “on” compared to “off”. The noise is especially pronounced over active centers. This is sketched in Figure 1a and b, where active sites are colored in rose. From the noise in the STM signal which is confined to a certain active area, we can assess the local reactivity.^[1] We report here the ability of the n-EC-STM technique to examine state-of-the-art model systems: Pt-based catalysts for the ORR and Iridium Oxide for the OER. An example of such a measurement on an IrO_x surface under OER conditions is shown in Figure 1c. An increased noise level can be seen when the reaction is switched “on” compared to “off”. In Figure 1d, height profiles in scan direction across the step edge marked in c are given. When the OER is “on” (blue), multiple spikes can be seen in the STM signal compared to “off” (brown).^[2]

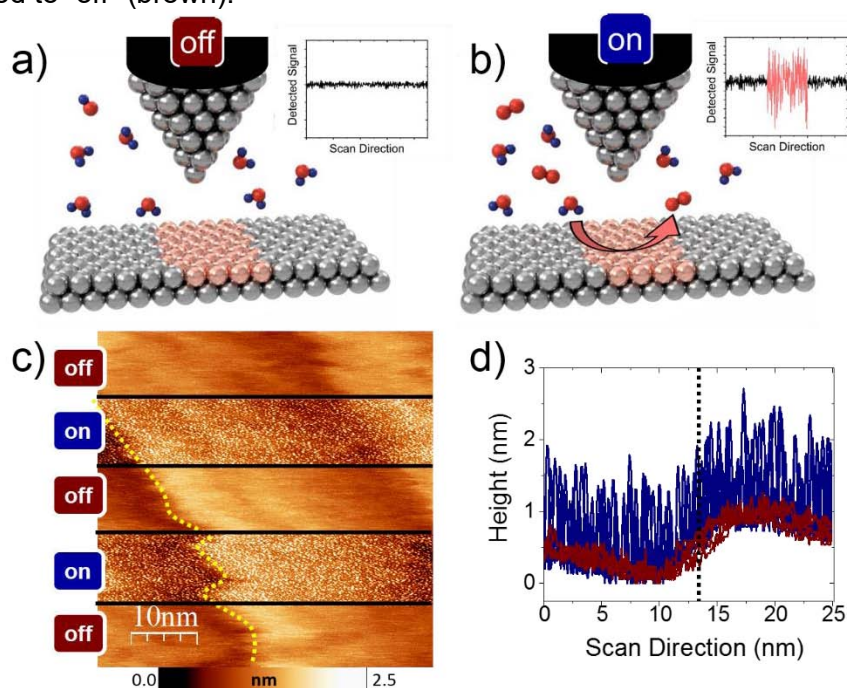


Figure 1. | a,b) Principle of the n-EC-STM technique to identify electrocatalytically active sites. c,d) n-EC-STM measurement on amorphous IrO_x in 0.1 M HClO₄. Reprinted from reference [2]. © 2021 Elsevier Inc.

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Highly Resolved Imaging of Active Sites for Carbon-Based Electrocatalysis under Reaction Conditions

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Due to the abundance and electrochemical versatility of carbon, it is becoming an increasingly popular material for electrocatalytic applications. Whether it is used as a support material, as a catalyst or even as a bifunctional catalyst, understanding at which surface sites reactions occur is of fundamental value. In this light, we employ electrochemical scanning tunneling microscopy (EC-STM) to in-situ evaluate the behavior of electrode surfaces and to identify the nature of the active sites.¹ The technique combines the monitoring of the sample surface on the nanoscale with the control of the reaction conditions. In consequence, experimental distinction between inactive and active sites of a catalytic system can be achieved by comparing the noise level of the respective recorded signal. If the scanning tip is positioned over an inactive site, the tunneling current will be stable. Over an active site, on the other hand, reactions occurring within the tunneling gap will influence the EC-STM signal which can be observed as locally confined noise features, superimposed on the surface morphology.

Here, we examine highly ordered pyrolytic graphite (HOPG) in alkaline and acidic media as a model system for carbon-based structures. In alkaline medium, we compare the activity of specific surface sites under oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) conditions (Figure 1a).² In both cases, predominantly steps and defects are active. However, in case of the OER, the terraces also play a role. For the hydrogen evolution reaction (HER) in acidic media, it was possible to identify individual active sites on the 'honeycomb' structured surface with down to atomic resolution (Figure 1b).³

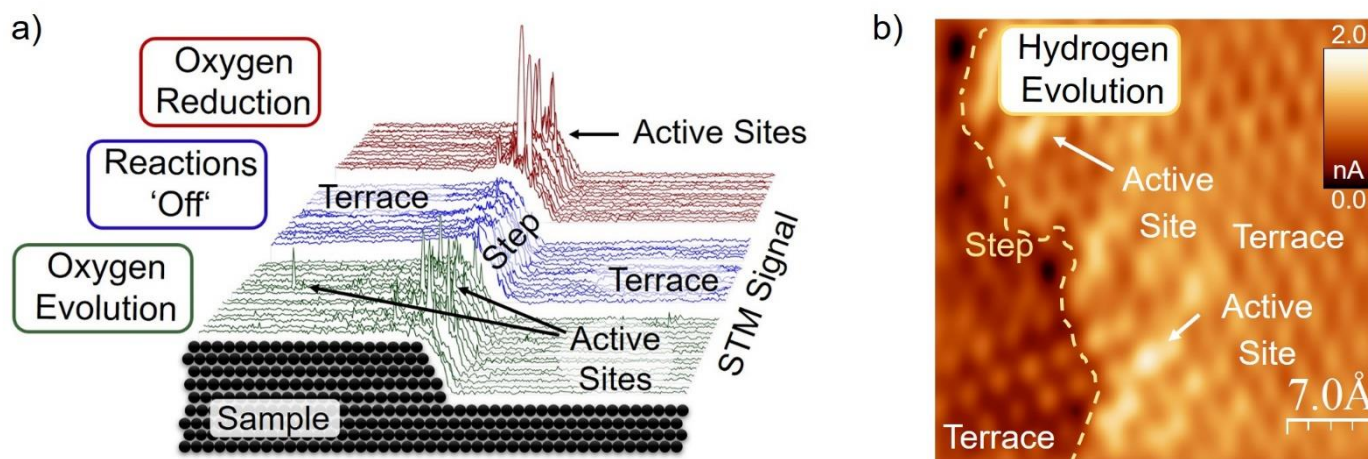


Figure 1: a) n-EC-STM measurement of a step under ORR (red) and OER (green) conditions, as well as during reaction 'Off' (blue). The most active sites in both cases can be found at steps, indicated by the distinct noise spikes at these positions compared to reaction 'Off'. Terraces are inactive towards the ORR, however, they do play a role in the OER.² b) Atomically resolved active sites on HOPG under HER conditions. Bright spots in the measurements indicate active centers. They can be observed predominantly at step edges and defects, while the basal plane (terrace) remains inactive.³

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A process approach for reactive power planning

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Due to the energy transition in Germany, the generation and load composition changes. For voltage stability aspects compensation systems and large-scaled conventional power plants satisfied the reactive power demand so far. In future, latter reactive power sources are deactivated and reactive power as a product for the system service *voltage maintenance* has to be procured by market-based mechanisms in order to fulfill the decisions of the European Commission. Therefore, grid control and planning processes for reactive power management have to be adapted or renewed.

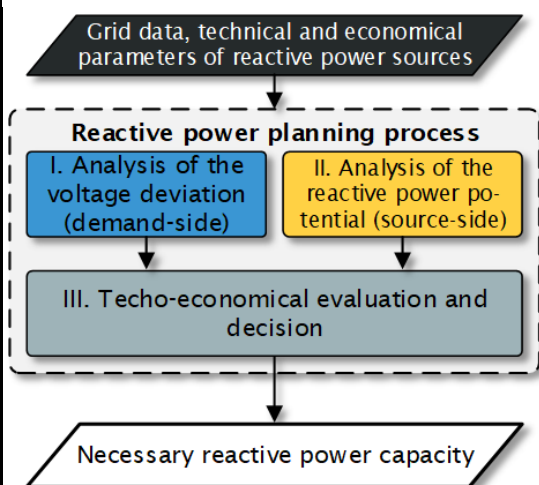


Figure 1: Reactive power planning process

For this investigation, different input data are necessary. Firstly grid data are required, which means a load flow simulation model of the grid including system-dimensioning P- and Q-data of the generators and loads, representative switching states and control behavior models of grid elements, e. g. Q(U)-control at energy plants or transformer tap controls. Secondly technical and economical parameters of existing and installable reactive power sources provide information to characterize the potential of the sources in sub-process II in its amount, availability, reliability, retrieval time, fixed and variable costs and also local technical efficiency.

The decision in sub-process III is based on two pillars: the analysis of the voltage deviation demand (I) and the analysis of miscellaneous reactive power sources (II). For the analysis of the demand-side (I) load flow and contingency calculations are carried out in order to determine the relative and absolute voltage deviations. The process user is able to define the voltage limits dependent on the system state and a tolerable probability for deficits (e. g. 2 %). The voltage demand can be evaluated for each grid node by duration-curves, see Figure 2. In sub-process II all relevant reactive power sources are technically and economically analyzed. In order to consider the local character of reactive power, $\partial V/\partial Q$ -sensitivity-factors are calculated to quantify the efficiency of the Q-injection of the sources to the demand nodes of Figure 2. In the last sub-process II the demands and sources are brought together and a decision is carried out by an optimization model by minimizing the overall costs with regard to the technical $\partial V/\partial Q$ -efficiency.

This work presents a new process approach for reactive power management, which is designed modularly and consists of three sub-processes (I-III), see Figure 1. The aim and the output of the process is the identification of the amount and the location of new reactive power sources (e. g. compensation systems) to fulfill the demand technically and economically efficient. The process is designed for a holistic application in transmission grids and subordinated distribution grids until grid level four and considers decentralized renewable energy plants as sources.

For this investigation, different input data are necessary. Firstly grid data are required, which means a load flow simulation model of the grid including system-dimensioning P- and Q-data of the generators and loads, representative switching states and control behavior models of grid elements, e. g. Q(U)-control at energy plants or transformer tap controls. Secondly technical and economical parameters of existing and installable reactive power

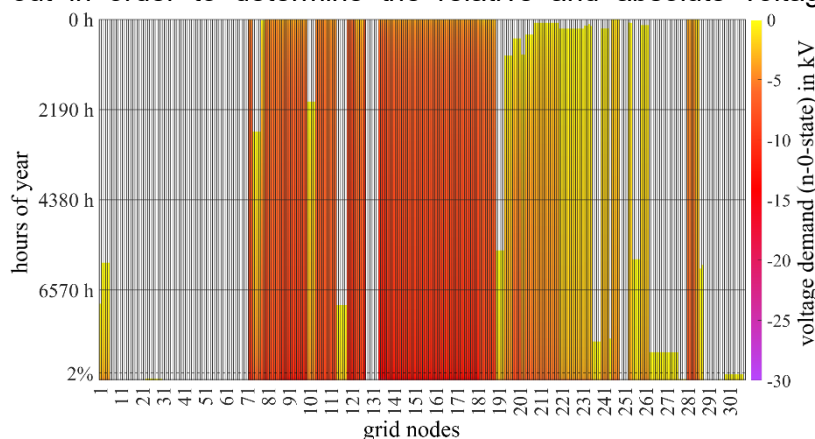


Figure 2: Duration-curve-heatmap of the voltage demand for the base case (n-0) of an exemplary transmission grid as a result of sub-process I

lemlab: A Toolbox for the Agent-based Design of Local Energy Market Applications

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In this poster we present *lemlab*, an open-source software toolbox for agent-based development and testing of transactive local energy market (LEM) applications. With the continually increasing penetration of fluctuating decentralized renewable energy sources (DRES) into modern power grids, LEMs present a potential solution to maintaining system stability by allowing the modern prosumer to participate in the liberalized market. Development of LEM applications requires extensive simulation and testing, with a significant portion of development time being devoted to the design and development of simulation tools. *lemlab* is a modular and

extensible simulation toolbox for the development and evaluation of LEM applications that provides pre-implemented scenario generation, agent-based trading strategies, a forecasting library, real-time capabilities, rolling-horizon convex optimization, as well as established and novel market clearing algorithms. This enables the rapid development of robust and real-world capable LEM applications.

Precursor engineering of two-step slot-die coated perovskite layers by TBP, MAI and DMSO addition

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The progress of hybrid perovskite materials has amazed the scientific community in the photovoltaic field, demonstrating a rapid progress in the performance within the last 10 years reaching above 25% power conversion efficiency. Now the investigation of ways to move from lab methods (e.g. spin-coating) to large-scaled production is required. Those methods include, e.g. roll-to-roll deposition, spray coating or sputtering. One of such roll-to-roll compatible methods is slot-die coating, which has several advantages: low waste of the used material, higher speed of production and possibility to print on a flexible substrate.

To reach highly homogeneous and defect-free, uniform films, two-step methylammonium lead iodide (MAPI) deposition is implemented. 4-tert butyl-perydine-assisted and methylammonium iodide-seeded solutions of lead iodide in dimethylformamide/dimethyl sulfoxide with different ratios as well as their combination are synthesized by slot-die coating with a home-built printer. Surface morphology is altered by addition of these solvents and those changes are investigated by SEM and XRD. Preferential orientation is studied by GIWAXS. Conversion to MAPI is tested and analyzed by XRD.

Results of this work can improve the quality of depositing PbI₂-films in two-step perovskite deposition method leading to full conversion of perovskite and better quality of final layer.

Visualising and weighting the multiple effects of building energy efficiency in conditional network structures

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Buildings play a versatile role in the life of humans and its surroundings. Occupants spend in average more than 90% indoors, buildings consume around 40% of our resources and energy. With increasing awareness, innovation and technology and the pressure of climate change, the quality and energy efficiency of buildings increased. However, A study by BPIE (2017) together with data of the EU Building Stock Observatory concluded that 97% of the building stock needs to be upgraded and only less than 3% achieve an energy standard of A. Motivation for deep building renovation is low and the high investment costs are mostly considered as investment with long payback periods. The reason for these unfavorable balances is the focus on only one main benefit of improving the energy performance of buildings: energy, respective energy cost savings.

The presented paper will extend this framework by introducing a complex network of multiple, wider benefits of energy efficiency, beyond energy cost savings. For the first time, this conditional network highlights the causal chain of direct and indirect effects of renovation measures in social, environmental, and economic means. It defines parameters, expected utilities and output formats which will support the quantification of these benefits and therefore enriches the long-term building renovation strategies with new arguments and monetized values which can even lead to reduced payback periods. The presented network is currently transposed into a Bayesian network which will be integrated into a comprehensive decision support tool.

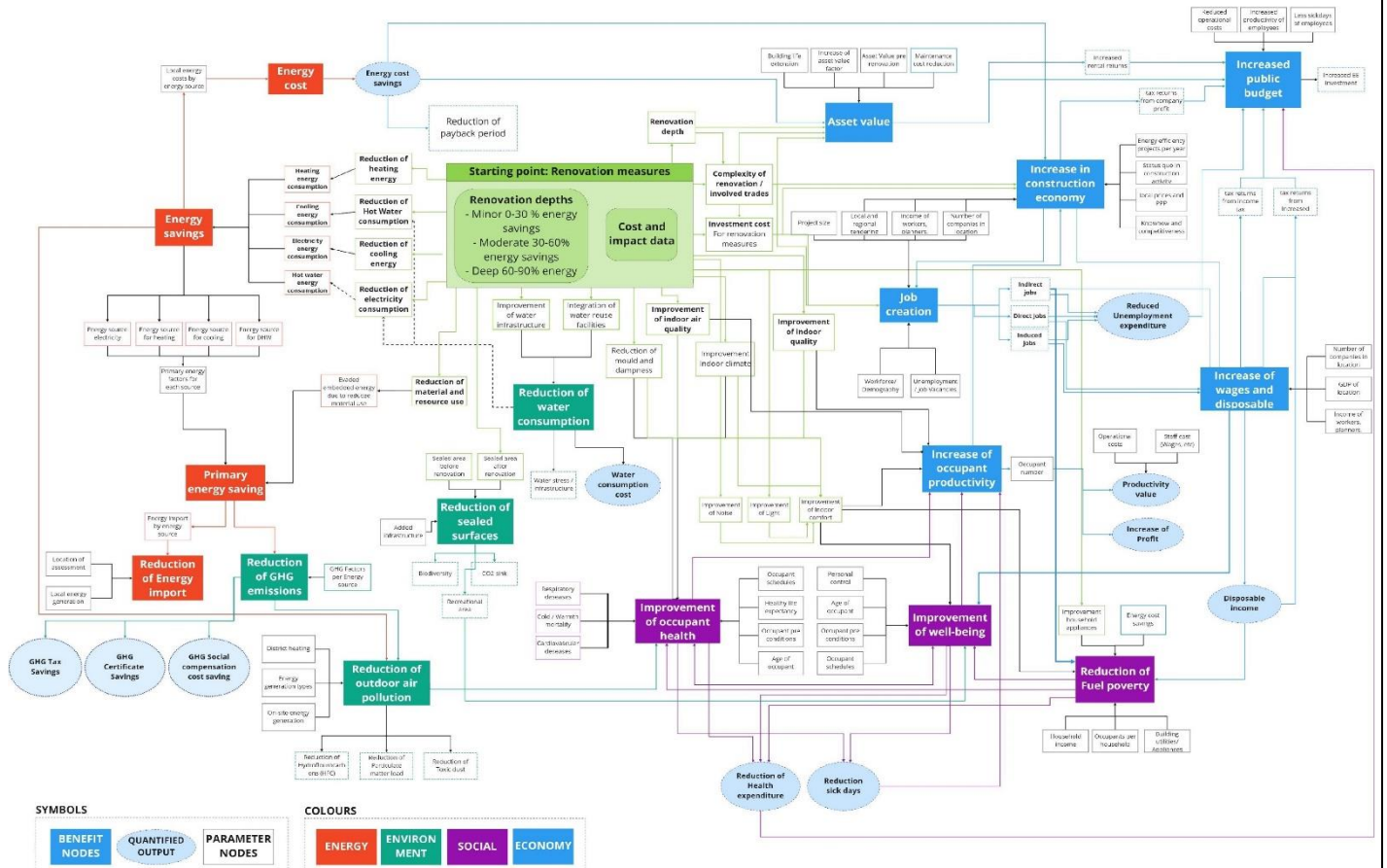


Figure 1: The network structure for the socio-economic assessment of building energy efficiency

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Impact and Allocation of Building Emissions

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In this research building emissions are identified and structured. Besides greenhouse gas (GHG) and CO₂-emissions these include further emissions with impact on people and the environment. Based on a systematic state of research a method to cluster buildings emissions and their occurrence is developed. Therefore, planners and decision makers are being helped in creating emission-free and positive buildings.

Global warming, pollution, environmental degradation, loss of biodiversity, waste and social conflicts count as the most important global challenges today. Facing these, a change and paradigm shift in the building sector as well as our society from less bad to positive has to be achieved. Since the building sector causes up to 30% of CO₂-emissions and 60% of generated waste in Germany, it plays a large role speaking of climate change mitigation [1, 2].

Although GHG are amongst the most important factors regarding global warming and climate change, there are no regulations for single buildings as there are for energy efficiency (e.g. EnEV/GEG in Germany). Moreover, there are lots of other emissions associated with buildings than GHG. In the following, these are identified and allocated in three different areas regarding their direct impact: global emissions, emissions by the building on the onsite environment (local) and emissions inside the building (interior). An overview is described below and also shown in Figure 1.

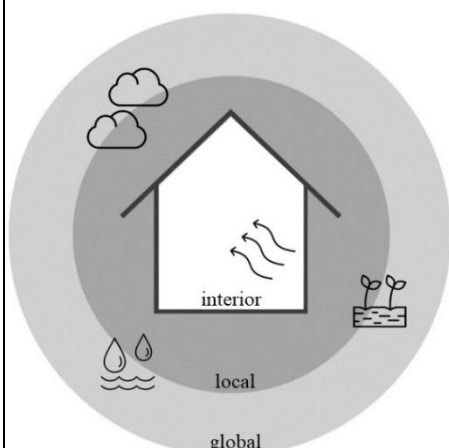


Figure 1: Spatial criteria for building emissions (own representation)

On the global scale, the most important gas regarding global warming is CO₂. Further GHG, e.g. methane and nitrous oxide, follow by a wide margin. [3] However, there are further emissions like ozone depletion, photochemical ozone creation, acidification and eutrophication which are taken into account when identifying a building's environmental impacts on terrestrial and aquatic habitats using the life cycle analysis methodology.

On a local scale emissions and other pollutants with risk to human health can be caused by burning fossil fuels or wood. Also, water and ground can be polluted by leaching from building materials and products such as roofs, facades or coatings.

Since humans spend up to 90% of their time inside of buildings, they get a lot in contact with interior materials including floorings, coatings or furniture. Therefore, (indoor) air quality and material health plays a significant role and urban air quality will be an important health issue in the future. [4, 5] Especially the selection and choice of building materials in early planning stages can contribute to a healthy indoor environment.

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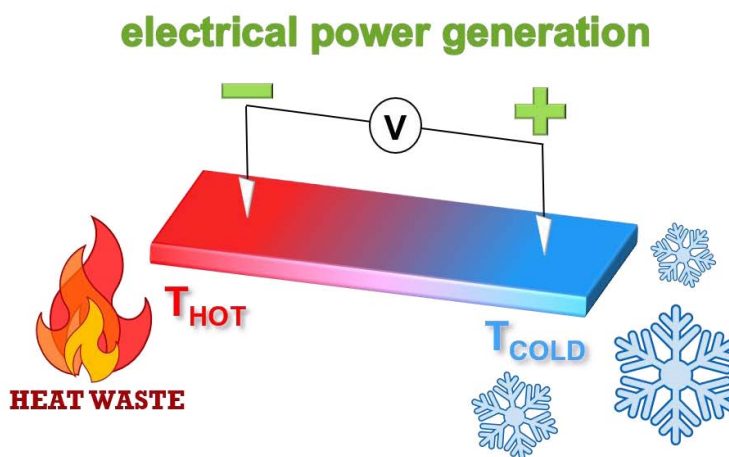
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Thermoelectric properties of organic semi-conducting polymer thin films during operation

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To fulfill the world's steadily increasing primary energy demand, current research is strongly focusing on the development and investigation of more sustainable energy sources. Renewable energy technologies like solar photovoltaic, hydro or wind power are nowadays already in commercial use. However, an issue that is often forgotten in the efforts to cover the energy demand is the huge wastage of energy as heat waste. Not only in industry, also in our daily life, like in our cars, mobiles, bad insulated buildings or even our own human bodies a lot of heat is created. As this heat mostly just dissipates unused into the environment, like that around 66 % of the global produced primary energy is just lost.[1] Therefore, it would be of immense importance if we are able to recycle this "lost energy" and convert the heat directly back into electrical power. For this purpose, thermoelectric (TE) materials provide a very promising way, as applying a temperature gradient on this kind of semiconducting materials leads to the formation of a usable electrical voltage. The hereby-underlying basic working principle is the so-called Seebeck effect.



Our research is focusing on organic thermoelectric polymers, as these own some advantages over the so far commercially used inorganic TE materials. As in, organic polymers are usually non-toxic, lightweight, flexible, and enable a large scale, low-cost solution based processability. However, the performance of these organic TE materials can so far not compete with the inorganic ones. Therefore, we are working on different treatment approaches to improve the TE performance of the non-toxic and water soluble organic semi-conductor PEDOT:PSS. With a treatment of ionic liquids (ILs), we have been successful in strongly increasing the conductivity and Seebeck coefficient of PEDOT:PSS thin films, which are both properties essential for a good TE performance.[2] With a variation of measurement techniques we investigate the morphology-function relation of the ILs treatment on PEDOT:PSS. Our current study is focusing on the stability of TE properties of these ILs treated polymer films under operation at elevated temperatures. It is important to understand the behavior of the films during long-term operation, and the thermal TE stability is a crucial condition for a possible future application.

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Tailoring ordered mesoporous titania films by introducing germanium nanocrystals for photoanodes

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Nanostructured titania films have attracted great attention due to their non-toxicity, low cost and morphology controllability, etc. These advantages enable them to be successfully applied in many fields, such as, photocatalysis, lithium-ion batteries and photovoltaics. Especially, anatase titania with interconnected network structures as well as a high surface-to-volume area is desirable as an electron transport layer in solid-state dye-sensitized solar cells (ssDSSCs) and hybrid solar cells. Until now, ssDSSCs based on interpenetrating titania networks can achieve high performance (up to 11.9%). Also, impressive efficiency of 25.2% has been reported in the hybrid perovskite solar cells. However, these advances all closely depend on the evolution of a superior sensitizer (dye molecules, quantum dots, perovskite-sensitized) or a hole-transporting material. Only a few researches exist targeting whether tailoring the titania could further improve the photovoltaic device performance. For example, Song et al. obtained more efficient titania photoanodes via incorporating with a presynthesised crystalline titania nanoparticles.^[1] Duan et al. designed TiO₂/GeO₂ nanocrystallite anodes with an attempt to increase the photogenerated electron density in the conduction band of the titania nanocrystallites and interference light intensity.^[2] In this study, we introduce dodecyl functionalized germanium nanocrystals (GeNCs) with a size of \approx 7-9 nm into the titania films for better solar cell performance.

Different weight contents of GeNCs are added to the titania sol-gel solution. During thermal annealing in argon at 500 °C, the templating block copolymer is combusted as well as the organic ligands on the surface of GeNCs. Finally, mesoporous TiO₂/GeNC composite films are obtained. Resulting surface and inner morphology changes are investigated by scanning electron microscopy (SEM) and grazing incidence small-angle X-ray scattering (GISAXS), respectively. The crystalline properties and elemental composition of the TiO₂/GeNC composite films are observed via X-ray diffraction (XRD), transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS), respectively. The optical properties are investigated by ultraviolet–visible spectroscopy (UV-Vis). Through the incorporation of GeNCs with varied weight percent, the optimized morphology and properties of TiO₂/GeNC composite films for solar cell application are studied, providing a promising photoanode candidate.

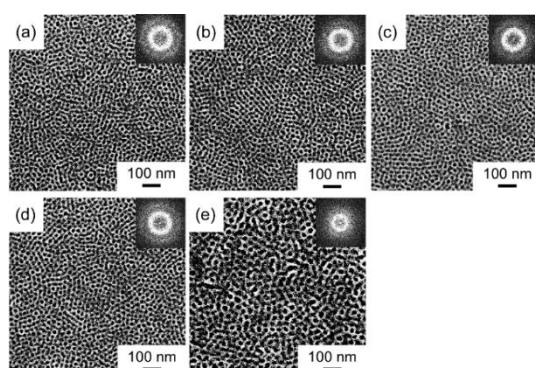


Figure 1. SEM images of the mesoporous TiO₂/GeNCs films after thermal annealing in argon at 500 °C: (a) 0 wt%, (b) 0.5 wt%, (c) 1.0 wt%, (d) 2.5 wt% and (e) 5.0 wt%.

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Economic control of hybrid energy system composed of wind turbine and battery

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An emerging approach for large scale grid integration of wind power involves hybridizing the wind energy system with batteries [1]. Operating such a hybrid plant in closed loop with an economically optimal controller can allow profit optimal operation, while adhering to the grid requirements and generating additional revenue by providing grid ancillary services [2]. The present work focusses on economic control and operation of a grid-connected wind turbine and Li-ion battery based hybrid energy system using an online economic nonlinear model predictive controller (ENMPC) in closed loop. The ENMPC directly balances between the revenue obtained from power generation and costs due to cyclic fatigue damage of wind turbine tower and cyclic capacity loss of the considered Li-ion battery while respecting the system constraints as well as those imposed by the electricity grid. The control variables are generator torque and pitch angle of wind turbine and charging/discharging power of battery.

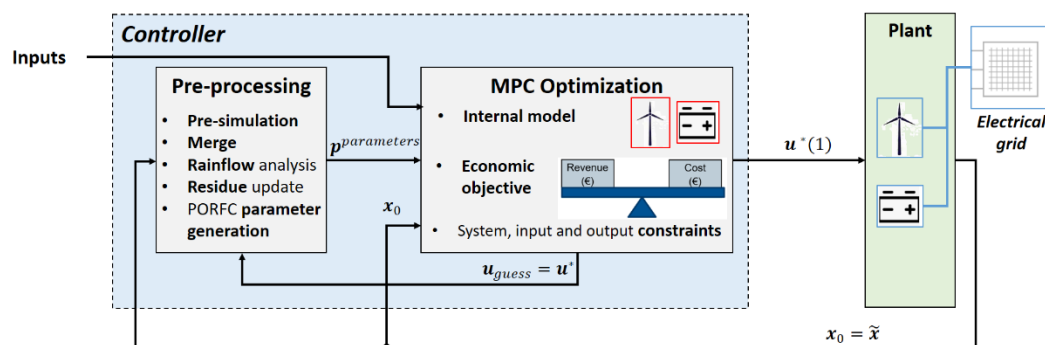


Figure 1: Closed loop simulation model for online economic control of wind turbine and battery based hybrid power plant.

The controller utilizes novel Parametric Online Rainflow counting (PORFC) formulation to explicitly and accurately formulate associated cyclic damages as an optimization objective [3]. This includes externalizing the cyclic fatigue evaluation (see

“pre-processing” block in Fig. 1) from MPC optimization step, to generate time varying parameters for accurate calculation of optimization sensitivities. To the best of our knowledge, a direct economic optimization by simultaneous consideration of wind turbine and battery damage against energy generation in an MPC framework has not been previously reported. This is possibly because the standard cyclic fatigue evaluation approaches, such as Rainflow algorithm, do not have an analytical formulation and contain algorithmic branches and loops resulting in a discontinuous output-behavior. This does not allow calculation of sensitivities required for standard gradient-based optimization techniques such as MPC.

The initial results for the formulated economic controller using novel PORFC algorithm show profit gain with suitable dynamic performance against a realistic base-case controller. Moreover, the explicit consideration of stress cycles from past in the controller results in enhanced economic performance. The controller also displays robustness against model disturbances such as wind speed. This motivates extending the approach towards more complex dynamical systems such as wind farm and solar plants based hybrid systems participating in modern grid ancillary services for obtaining profit optimal dynamic operation.

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Stable Colloidal Quantum Dots Inks Enable Infrared Solar Cells via Printing

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Colloidal quantum dots (CQDs) have generated great interests in the various optoelectronic devices in view of their size-tunable bandgap, low-temperature solution processability. Lead sulfide (PbS) CQDs, with strong absorption coefficient and large Bohr radius, enable solar cells to harvest infrared photons of the solar spectrum beyond the absorption edge of crystalline silicon and perovskites. Recently, the CQD ink from solution ligand exchange[1] allow the active layer in a single step by large-scale manufacturing processes, which has been demonstrated to realize high-performance solar cells[2]. However, the unstable amine solvent (i.e., n-butylamine) for CQD ink causes QDs' surface etching and degradation, and its low boiling point is incompatible to scalable fabrication techniques.

The excellent passivation, high charge transport and good colloidal stability in ligand exchange are required for high quality CQD ink. Moreover, various solvents and their mixes are paramount of importance in the ink rheological properties such as boiling point, polarity and concentration, affecting the optoelectronic properties of the printed films via slot-die coating. Herein, we focus on the solvents for ink deposition using meniscus guided slot-die coating. We employ N-methyl-2-pyrrolidone (NMP), N-methylformamide (NMF) and N,N-dimethylformamide (DMF) to mix respectively with n-butylamine(BTA) in appropriate volume ratios, studying the solvent effect of CQD ink on carrier transport and morphology control in the final film and CQD solar cell performance. With scanning electron microscopy (SEM), atomic force microscopy (AFM), and grazing incidence small-angle X-ray scattering (GISAXS), the surface morphology and inner structure of printed films is studied. We study their charge carrier dynamics with transient absorption (TA) spectroscopy, and their optical properties with photoluminescence (PL), UV/vis absorption spectroscopy. In addition, we fabricate the infrared solar cells based PbS CQDs film via slot-die coating and measure external quantum efficiency (EQE) and the corresponding the power conversion efficiency (PCE).

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Optimization and Restructuring of District Heating Networks

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Objective

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). Strategies to reduce losses in rural DHNs are analyzed using the example of two existing ones. The aim is to improve DHN with low-investment measures. This should enable them to be operated cost-efficiently in the future.

The catalog summarizes already published studies and includes the results of the ongoing project investigations. The economic expenditure and the potential savings of the respective measure are evaluated. Besides, the retrofitting of already installed district heating substations (DHSs), an innovative operating strategy as well as the integration of existing renewable sources into the DHSs will be investigated.

District Heating Substations

The hydraulic setup of DHSs has a high influence on the return temperatures. Significantly lower return temperatures have already been achieved for multi-family houses through hydraulic modifications (Stadtwerke München et al., 2014). Improved control strategies for DHS can also reduce return temperatures and volume flows in the DHN (Gustafsson et al., 2010; van Oevelen et al., 2018). In the current project the existing DHS are being upgraded to be cost-efficient. Typical consumers in the specific DHN are single-family houses. Therefore, the scope of costs is smaller than for other objects.

Central Operation Strategy

An innovative operation strategy will be examined on a simulation-based method. Schedule-based operating strategies are examined, to lower feed temperatures on an annual average (Euring, 2017; Leoni, 2018). Achieving this, the DHS will be upgraded with a controller that can communicate with the heating center of the DHN.

Optimized Integration of Renewables

In Germany, decentralized heat sources like solar thermal systems are common, especially in rural areas. Decentralized heat sources have a negative impact on the efficient operation of DHNs. Hence, an overall operating strategy is to be developed and investigated.

Results

A preliminary evaluation of the economic and ecological benefits of optimization measures is presented.

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Structural Analysis of Co-precipitated Ni-Al Catalysts for CO₂ Methanation

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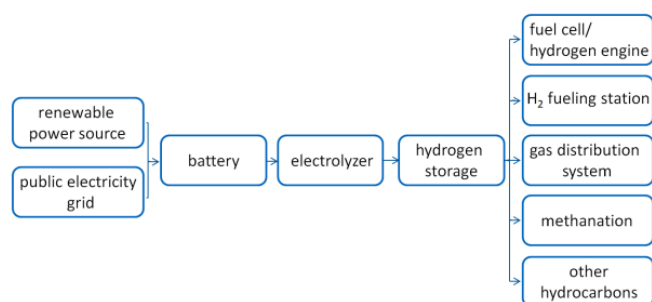


Figure 2: Main components of a power-to-gas system. Adapted from [1].

Due to the rapid population growth and continuously increasing energy demand, the provision of energy from renewable sources is inevitable with regard to combating global warming.[1] However, effective ways of storing the energy obtained have to be found. The so-called power-to-gas (PtG) concept is a promising solution for this. Hereby, the energy from renewable sources is converted into hydrogen *via* electrolysis of water and is then converted with CO₂ into methane as part of the so-called methanation.[2] 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. Yet, their detailed structural changes remain open questions. For that purpose, we synthesized catalysts with different Ni/Al ratios ($n_{\text{Ni}}/n_{\text{Al}} = 5 - 0.33$) which were calcined in synthetic air and afterwards activated under H₂ atmosphere. The materials were characterized in detail using various techniques. Their aging behavior was investigated using the methanation reaction as a model.

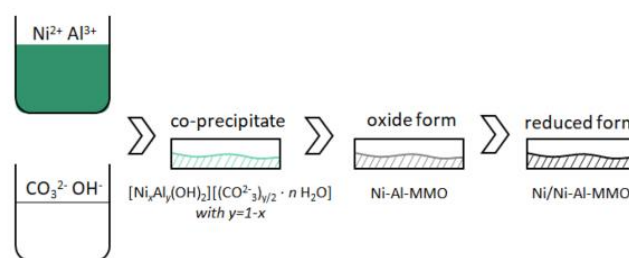


Figure 1: Different stages in the preparation of co-precipitated Ni-Al catalysts. Adapted from [3].

The co-precipitated materials feature a hydrotalcite-like structure showing an increasing basal interlayer distance with rising Al content. After calcination, this structure is transformed into a Ni-Al mixed metal oxide (MMO). As coupling of XRD with TPR showed, the calcined materials feature the coexistence of a Ni-rich crystalline phase as well as an amorphous Al-rich phase. Referring to the sample with $n_{\text{Ni}}/n_{\text{Al}} = 1$, according to TPR measurements, Ni⁰ originates partly from the crystalline NiO phase and partly from amorphous Al³⁺. Possibly, the resulting lower Ni/Al ratio in the oxidic phases leads to the formation of coordinately unsaturated O²⁻ sites, giving rise to medium basic sites.[4] CO₂-TPD reveals that the basicity of the investigated materials is mainly caused by OH groups weakly binding CO₂. During activation at 485 °C, *in situ* medium and strong basic sites are formed. After aging under CO₂ methanation conditions, the Ni/Al ratio in the bulk of the crystalline oxidic phase is further decreased, provoked by the high partial pressure of steam. Accordingly, X-Ray PDF confirms the decrease of the Al-O and Al-Al bond distances. In addition, near-ambient pressure XPS measurements gave rise to the formation of Ni hydroxyl species on the catalyst surface which could be another deactivation pathway and is possibly accompanied by a loss of basic surface sites and BET surface area.[5,6]

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Non-destructive quantification of lithium and electrolyte losses in Li-ion batteries

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Modern lithium-ion batteries display a remarkable deterioration under extensive cycling, where they lose a part of their capacity and power. Such losses are caused by a variety of side reactions occurring during cell operation like the formation of the solid-electrolyte interphase (SEI), loss of active lithium, drying out of the cell etc. These side reactions occur at local places in the cell, which result in the development and promotion of heterogeneous states (e.g. lithium distribution in the electrode materials). The loss of active lithium is typically related to the growth of the SEI during cell cycling, whereas the quantification of the electrolyte losses during the cell operation (vs. cell fatigue) is not reported.

Classical *ex-situ* characterization of the cell components is usually supplemented by the extraction of the cell materials and therefore by the destruction of the isolated state of the cell. This leads to unavoidable changes in the state of the materials due to evaporation of electrolyte, oxidation of electrodes, etc. occurring during *ex-situ* studies. The *per se* non-destructive methods based on high energy X-rays or neutrons are typically not capable to quantify the amount of liquid electrolyte with needed accuracy.

It has been found that at temperatures below 260 K a long-range ordering corresponding to frozen state is built up in the series carbonate esters mixtures. This long-range order has been found

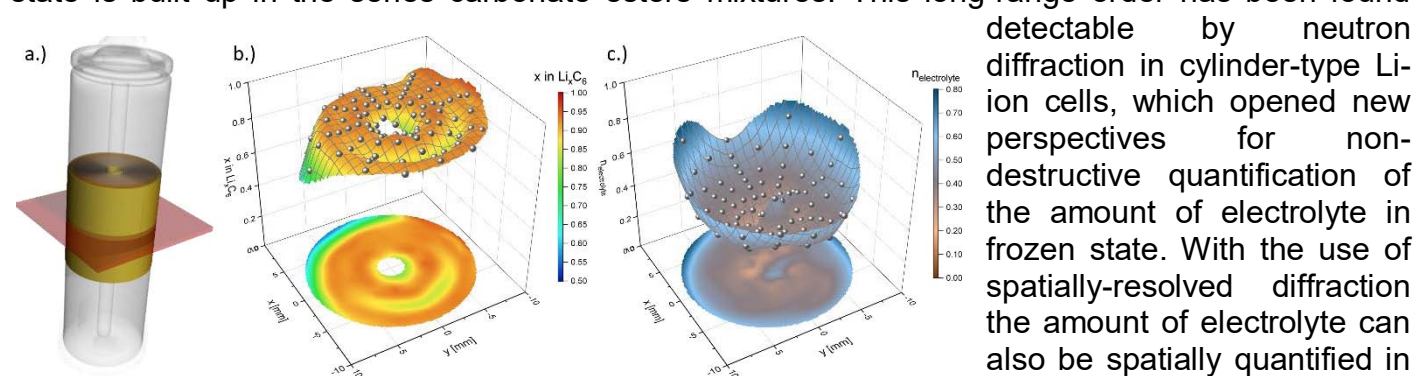


Figure 1 a) Measuring volume of a 18650-type lithium-ion battery with corresponding b) lithium and c) electrolyte distribution investigated with in-situ neutron powder diffraction

detectable by neutron diffraction in cylinder-type Li-ion cells, which opened new perspectives for non-destructive quantification of the amount of electrolyte in frozen state. With the use of spatially-resolved diffraction the amount of electrolyte can also be spatially quantified in different parts of the cylinder-type battery. Besides this a non-destructive quantification

of lithium inside the graphite anode was performed and compared to the relative concentration of electrolyte (Figure 1). The evolution of lithium and electrolyte contents as well as their spatial distribution were determined for a batch of cells cycled for a different number of cycles, where different states of fatigue were stabilized.

A combination of electrochemical characterization, X-ray computed tomography and neutron diffraction studies is applied to a batch of 18650-type cylinder cells based on NCA|C chemistry, where high-resolution neutron diffraction independently reveals a direct correlation between the volume-averaged losses of active lithium in the graphite anode and those of liquid electrolyte. The spatial distribution of active lithium and electrolyte losses have been found to exhibit a non-trivial relationship to the complex dynamics of capacity fading indicating rapid development of heterogeneous states.

In-situ study of ionic liquid additive on structure, composition and overall performance of perovskite solar cells

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Perovskite solar cells (PSCs) are one of the most promising photovoltaic technologies and reached

a certified 25.2% efficiency owing to their tuneable bandgap, high carrier mobility, long diffusion length and so on.^{1, 2} However, defects can be formed in the fabrication process regarding the nature of solution processing and rapid crystal growth of perovskite thin films, thereby inducing the increased trap density and the decreased performance of PSCs. In this work, an ionic liquid additive is used to eliminate the aforementioned defects, and a pinhole-free and fully coverage film was obtained, leading to an enhancement of power conversion efficiency (PCE) and long-term stability. The improvement of PCE and stability can be ascribed to the enlarged grains and suppressed ion migration with the addition of the ionic liquid. In particular, the influence of the ionic liquid additive on the structure, morphology of perovskite film and also long-term stability of devices is studied using *in situ* grazing incidence wide-angle X-ray scattering (GIWAXS).

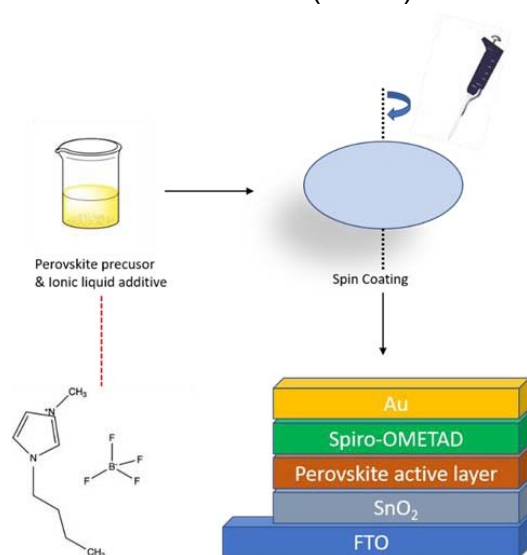


Figure 1: Schematic illustration of the preparation process of perovskite solar cells

Characterization of grid-side requirements for flexibility measures in power system planning

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The turnaround in the German energy policy is leading to an increasing expansion of renewable energy sources (RES) in the distribution grid. Also, a rising demand for electromobility can be expected, which may contribute to a further exhaustion of the permissible voltage ranges and line loads. In order to increase the absorption capacity of the distribution grid, various solutions have been developed and established in the past. An additional tool for resolving grid bottlenecks and voltage problems is the time shifting of feed-in and consumption loads in the medium-voltage level. These so-called flexibility measures are not yet state of the art. In order to provide a high benefit by contributing to an efficient saving of assets, they must be implemented in the grid planning.

The investigation of several urban and rural grid areas shows, in addition to the expected differences in the level of power demand due to the respective grid topology, a very individual behavior with regard to the temporal distribution of limit violations. Therefore, a characterization transferable to all grid areas is introduced to describe the grid-side flexibility requirements. For this purpose, first the minimum and maximum reference power of a provider $P_{Ref,min}$ and $P_{Ref,max}$ have to be determined, between which the respective consumption load/supply has to be located at any time. This reference power range can vary, for example, depending on the season, the day of the week and the time of day, and makes it possible to infer the required or available flexibility power ΔP_{max} (load-increasing) or ΔP_{min} (load-reducing) (see Figure 1).

The flexibility measures can be specified in terms of time via the specification of operating time windows $\Delta t_{w1,w2,\dots}$ with the start times $t_{w1,w2,\dots}$. From the grid planning point of view, a provider must basically be able to provide its offered flexibility for the entire duration and

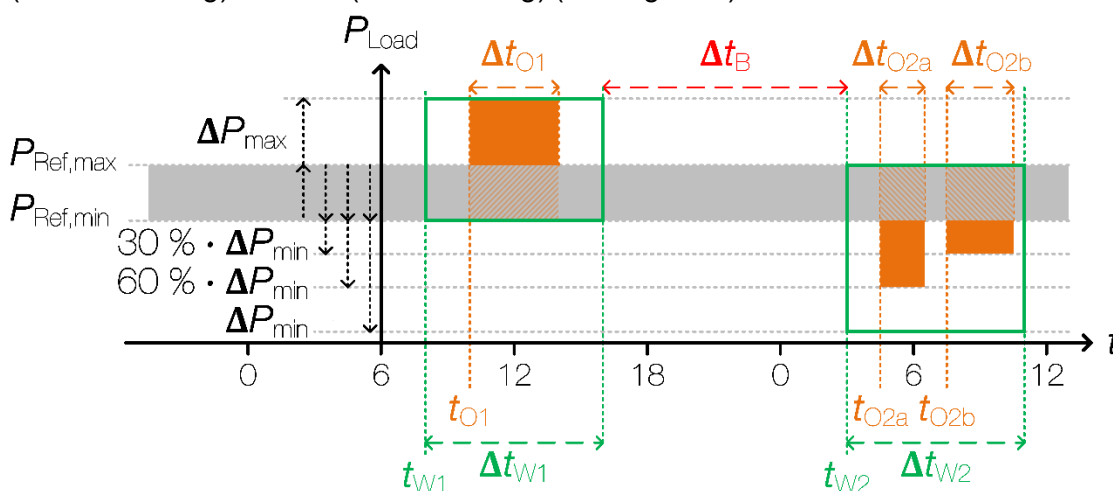


Figure 1: Characterization of the grid-side flexibility requirements

in the full amount of power. The actual operating times $t_{01,02,\dots}$ and operating durations $\Delta t_{01,02,\dots}$ only arise during grid operation. It is also interesting whether the flexibility power can be called up in a fixed, staged (30/60/100 %) or variable manner and whether the flexibility calls can potentially be split within the operating time windows. For the planning on the grid and supplier side, it must also be determined which break Δt_B is between two operating time windows and with which frequency/probability of occurrence the flexibility calls appear - in addition to checking the technical requirements, this also influences the economic calculation.

The characterization can be used, for example, to analyze how much flexibility energy must be deployed to fully resolve voltage limit violations. Another possibility is to solve only a part of the problem by using flexibility and to rely on a combination with feed-in peak capping instead. This approach is particularly useful if there is not enough flexibility potential on the supplier side or if the full amount cannot be used economically.

Impact of CO₂ 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 charge and discharge processes is the key point to promote Sb-based anodes to practical applications. Carbon dioxide (CO₂) 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 CO₂ and carbon, CO₂ 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, CO₂ activation is also a fast and facile method which can perfectly adapt to the fabrication system. As a result, after CO₂ 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 CO₂-activated Sb/C nanohybrid as sodium-ion battery anode is also demonstrated, showing a good electrochemical performance.

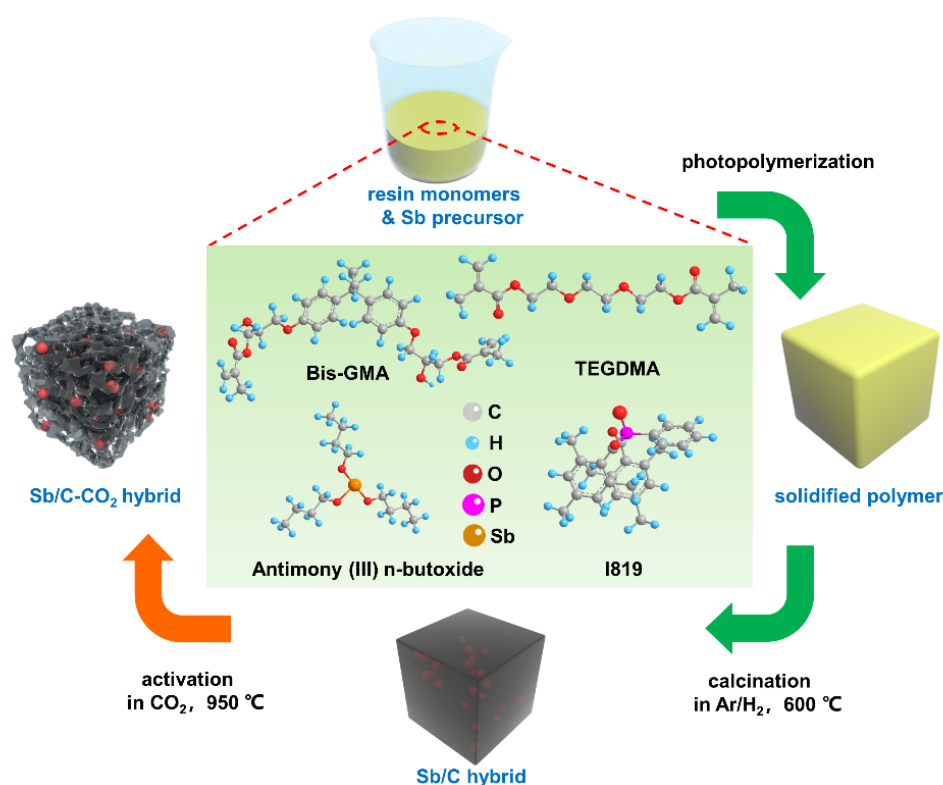


Figure 1: Schematic illustration of the preparation process of the Sb-based nanohybrids without CO₂ activation (Sb/C hybrid) and with CO₂ activation

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Analysis of Total Cost of Ownership of Electric Vehicles compared to Conventional Vehicles for different User Types in Germany

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The transport sector is one of the main emitters of climate-damaging CO₂ and has the potential to contribute substantially to the fight against climate change. A major lever to reduce emissions in this sector is the electrification of transportation - especially of private cars. Policymakers worldwide have introduced in recent years targets to increase electric vehicle adoption in their country. Germany itself has the target to raise its electric vehicle fleet to 7 - 10 million until the year 2030 from 0.3 million nowadays. Despite that the adoption of electric vehicles is growing, many consumers are deterred by the high initial purchase price of these cars and often have limited knowledge of the potential cost savings during operation. The total cost of ownership concept (TCO) creates full transparency on all costs occurring during the ownership of a car for the consumer and can be adapted to specific user types.

For this reason, this paper aims to contribute to the existing TCO research with an analysis of the TCO for Germany in 2020 with different typical user profiles. To be representative of the German market, we selected for our analysis different vehicle segments and propulsion types and included actual cost data. We applied the current subsidy scheme for low emission vehicles in Germany and compared it with the previous subsidy scheme introduced in 2016. Furthermore, we introduced 9 different user types categorized by annual driven distance and residential user type to investigate TCO differences by user profiles.

Our results show that even with the lower subsidies from 2016, full electric vehicles are already a favorable economic option in the compact segment and plug-in hybrid vehicles in the SUV segment. The increased subsidy scheme in late 2020 has not significantly shifted the economic ranking of different propulsion types in the respective segments, but without question accelerated electric vehicle sales. However, it even can be questioned if a different incentivization could have been more cost-efficient and on the same time could have changed some unfavorable conditions like the economic better position of the plug-in hybrid vehicle compared to the full electric vehicle in the SUV segment and the better economic position of internal combustion vehicles compared to low emission vehicles in the small vehicle segment.

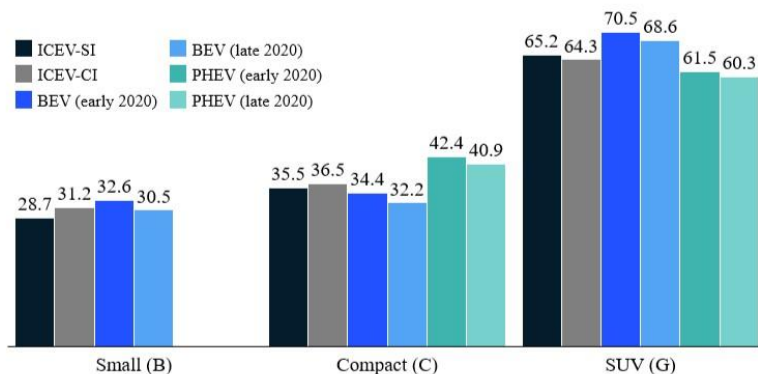


Figure 1: Total cost of ownership for sub-urban user with average annual driven distance (15,000 km) for selected segments and propulsion types with subsidy scheme from early and late 2020 [EURcent/km]

The findings show that while the purchase cost of the vehicle is the main cost category, insurance, parking and fuel costs are the main differences between residential user types. However, the differences between the user types are currently marginal and do not shift the economic ranking of vehicles between different user types. With the adaption of these costs through for example a change of parking costs or a larger offering of low-priced electric vehicle insurances in specific areas, it is possible to steer vehicle costs by specific user types. This would enable for example policymakers to steer incentives to areas with high impact like the reduction of emissions in traffic-dense urban areas.

Impact of Smart Home on the Green Deal

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In 2019, the Green Deal was adopted by the European Commission¹. The aim is to minimize greenhouse gas emissions to zero by 2050 and to become completely climate neutral. To achieve this goal, the construction sector must also make its contribution to a climate-neutral environment. This is because a great deal of energy and CO₂ emissions can be saved not only during the construction stage, but also during use stage. All this is to be achieved with the help of building automation. Intelligent building automation can save a lot of energy in buildings, in terms of energy consumption for heating, cooling and electricity. Furthermore, life-cycle-based costs can be minimized, because such systems have much more far-reaching advantages.

A study on the user behavior of smart homes in 2020 by Bitkom e.V. came to the conclusion that a higher quality of life and more energy efficient living are among the main aspects of users and prospective buyers. Furthermore, a specially designed and conducted survey clearly showed that the indoor climate has a tremendous impact on employees and is also very important to them.² However, it still keeps many off from buying a smart home system because the initial investment is too expensive. Therefore, in this study a profitability calculation is conducted, to analyze the amortization time of smart home systems and their impact on a healthier indoor environment.

In order to carry out the amortization calculation, considering all relevant influencing factors (e.g., energy saving, more effective employees, healthier employees), the focus is on the two aspects of energy efficiency and indoor climate. Thus, the introduction and later staggering of the CO₂ tax of the federal government plays a role and is included. Likewise, the topic of comfort of employees in office buildings is considered according to the workplace directive.

In terms of operating costs, building automation can so save 29% of heating energy and 48% of electricity consumption.³ A good indoor environment with adequate air exchange rate, appropriate and adjustable room temperature, good interior design and no air pollution can increase the effectiveness and productivity of employees by 23% - 34%.⁴ In addition, the health of employees is positively influenced, thus reducing absenteeism by 5%.⁴

This amortization calculation is carried out using a net present value method based on a real practical example. The office building of the company Nelhiebel Elektrotechnik GmbH, newly constructed in 2018, is used for this purpose. The entire building was equipped with the latest technologies and high-quality components across all trades. Through interfaces to protocols such as BACnet, DALI, Modbus, ZigBee, etc., all trades are integrated into the KNX bus technology. This variety of building technology and outstanding building automation was not only certified according to the KfW-40 standard, but also awarded by the ZVEH and Wirtschaftsinitiative Smart Living in 2020 by winning the Smart Living Professional Award in the category "Application in own company".

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³ Siemens. *Energieeffizienz in der Gebäudeautomation*;

⁴ Krödel, M. (2020) *Der Einfluss von Smart Building auf Wohlbefinden und Produktivität von Mitarbeitern im Büro*; Ottobrunn: IGT-Institut für Gebäudetechnologie

New Insights on Ni-Al Catalysts for the CO₂ Methanation by X-Ray Photoelectron Spectroscopy

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The production of synthetic natural gas (SNG) through the methanation of CO₂ with H₂ has gained wide interest as a way to store and transport energy from renewable sources. As part of the power-to-gas concept the highly exothermic Sabatier reaction [1] plays a crucial role in the establishment of a CO₂-neutral energy sector. For industrial applications, Ni-Al catalysts are well established for that reaction.

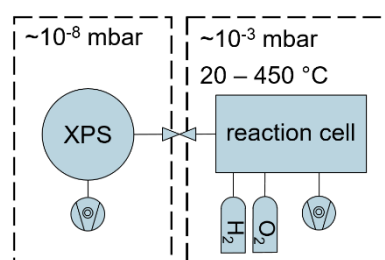


Fig. 1: Lab XPS with reaction cell.

Using X-ray photoelectron spectroscopy (XPS), various Ni-Al mixed metal oxide catalysts were analyzed. The experimental setup (*cf.* Fig. 1) allows to characterize changes on the catalysts surface upon various reaction conditions *quasi-in situ*. Aiming at characterizing the catalyst surface after calcination, during activation and upon re-calcination, qualitative and quantitative findings were derived from XP spectra.

Based on Ni 2p core level spectra, we were able to assign Ni²⁺ species on surfaces of various impregnated and co-precipitated catalysts in the calcined state to either a mixed metal oxide NiAl_xO_y or bunsenite (NiO). Deconvolution of the Ni 2p_{3/2} spectra revealed the detailed surface compositions of the analyzed samples.

After activation of the co-precipitated catalyst, the Ni²⁺ surface species are almost completely reduced to Ni⁰ (*cf.* Fig. 2A). Quantification of the data further revealed the accumulation and formation of Ni⁰ nanoparticles on the surface. These findings are in good agreement with XRD data in literature [2].

A pressure gap could not be detected as XRD revealed the same Ni⁰ particle formation for the catalyst activated in a common reactor (*cf.* Fig. 2B). These findings ensure that the bulk is affected in the same way, independent of the total pressure. As a result, we conclude that activation in our ultra-high vacuum-based setup and subsequent XPS analysis provide representative results for the surface composition of technical Ni-Al catalysts and their surface changes upon activation.

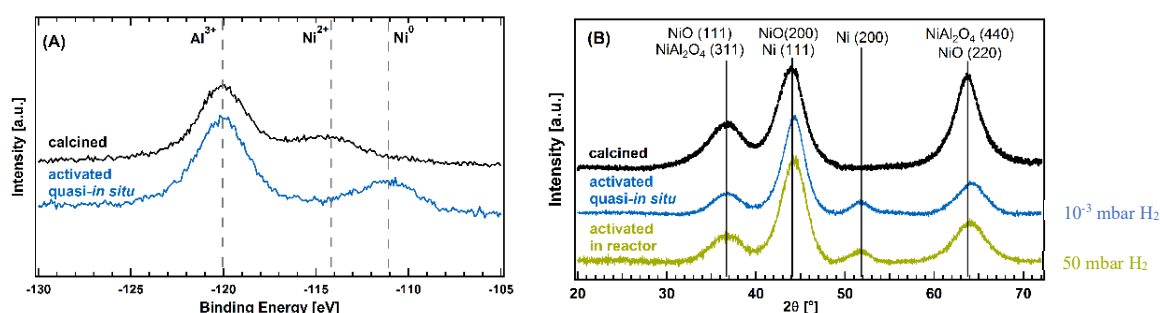


Fig. 2: Co-precipitated catalyst ($n_{Ni}/n_{Al} = 1$): (A) Core-level spectra of the Ni 3s/ Al 2s region in the calcined state (black) and after activation (blue), (B) X-ray powder diffractograms in the calcined state and after activation in the *quasi-in situ* setup (blue) and in a technical reactor (green).

A re-calcination treatment in the UHV setup directly following the activation leads to the re-formation of oxidic Ni on the surface. Also a spreading of the Ni particles was observed, which were rebuilt as before upon a further re-activation treatment.

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Surface Area Evolution of Li-and Mn-rich Cathode Materials for Lithium-ion Battery: Comparative Investigation on Dense vs. Porous Morphology

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Abstract

Li-and Mn-rich (LMR) layered oxides have received special attention as one of the most promising next-generation cathode active materials (CAMs) for lithium-ion batteries due to their high energy density and low cost [1,2]. State-of-the-art LMR materials typically possess a loosely packed, porous morphology. However, a densely packed morphology can potentially achieve enhanced volumetric, and gravimetric energy densities as well as improved processability during calendaring of electrode sheets [3]. But our previous investigation showed an different electrochemical performance of dense CAMs- compared to the established porous CAMs, which is predominantly caused by their difference in surface area, and bulk strain. For example, dense CAMs, which has 5 times lower surface area than porous CAMs presented inferior performance due to its limited contacted area with electrolyte. Although the surface area turned out to be one of the key parameters to determine the performance of LMR cathodes, the correlation between surface area evolution and morphology during cycling has not been clarified yet. In this work, we conduct comparative tracking of surface area evolution by Kr-BET analysis as a function of electrode compression, initial cycling, and state of charge (SOC). Effects of CAM surface area on electrochemical performance are additionally analyzed with rate capability test. The results confirm that surface area does not show meaningful change until the 2nd cycle at discharged state, relative to the pristine CAM. However, a significant increase of surface area (-up to 60%) is observed at high SOC (charged states); Especially porous CAMs show a 20% higher surface area increase than dense CAMs. During the rate capability tests, the capacity gap between the porous and dense CAMs becomes considerably reduced when current density is normalized by the actual surface area of each CAMs.

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Sustainable Energy Supply Concepts for University Buildings

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In order to limit climate change, Germany has set itself the goal of achieving climate neutrality by 2050. To achieve this goal, the building sector plays a key role, as it is responsible for about one third of final energy consumption and greenhouse gas emissions. [1] [2]

As part of the NuData Campus project (www.nudata.de), the feasibility of climate neutrality in the operation of university buildings is being investigated on the basis of the building stock of the HM Hochschule München University of Applied Sciences. The aim is to develop a life-cycle based climate-neutral energy supply concept, taking the special requirements of educational buildings into consideration. This is intended to provide a basis for maximizing the potential of practical implementation of climate neutrality in operation for university buildings.

For the development of the concepts, a combination of a differentiated evaluation methodology is used. Sustainable evaluation criteria based on a life cycle assessment (LCA) as well as building performance simulations are applied.

First, an analysis of all current energy supply systems will be made with regard to their theoretical and general suitability for climate neutrality. This includes data on efficiency, but also data that consider the life cycle of a concept. Data from the current standardization as well as from the Ökobaudat will be used. [3] [4] [5] [6] [7] First of all, a catalog of criteria is defined for evaluation, which identifies the various factors by which a climate-neutral building operation is influenced. The focus is on the transferability to other buildings.

The systems are evaluated according to the following criteria:

1. Feasibility: It is necessary to weigh up whether an energy supply concept for a building is fundamentally feasible. This is a knock-out criterion. If a supply concept is not fundamentally feasible, it is not considered further (e.g., ground collectors in inner-city areas because there is not enough space available)
2. Efficiency: The efficiency of the individual systems is compared in an appendix of characteristic values. These include: Efficiency, annual utilization factor, seasonal performance factor, coefficient of performance, energy efficiency ratio and seasonal energy efficiency ratio
3. Resource use: The resource use for the life cycle phases A1-A3 (manufacturing phase or production), B6 (energy use during use) and C3 (waste treatment) is considered
4. Environmental impact: The environmental impact is considered for the life cycle phase A1-A3 (manufacturing phase or production), B6 (energy input during use) and C3 (waste treatment)

The systems are then evaluated and selected on the basis of these specific criteria in order to identify the techniques that are fundamentally most suitable for the required purpose. This procedure is carried out using a representative building of the HM Hochschule München University of Applied Sciences.

In order to consider the actual functionality of the selected heating concept in more detail, an energetic-thermal simulation is carried out. For this purpose, the technologies are implemented in the simulation software IDA ICE. Finally, the concept that emerges as the most advantageous variant is to be transferred to the detailed building model.

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Influence of solvent composition on performance and morphological properties of low cost organic solar cells

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Solar power is one of the fastest growing renewable energy sources to supply the continuously growing global demand for clean power. Currently, silicon-based photovoltaics (PVs) make up the majority of the commercial market for solar cells and demonstrate regularly module efficiencies of over 20%. Yet, their energy intensive production and therefore long energy payback time motivate the search for novel materials, which might complement silicon-based PVs.

Especially organic solar cells have recently gained growing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their production. Due to their highly tuneable optical properties and their solution-based manufacturing techniques, they exhibit a wide variety of potential applications, ranging from semi-transparent to flexible solar modules.

However, the organic solar cell manufacture relies heavily on the use of halogenated solvents, whereas organic solar cells made with more environmentally friendly solvents often suffer from major performance reduction. This is largely attributed to the changes in the nanoscale morphology of the polymer donor materials and the small-molecule acceptor materials that form during the drying process of the wet film [1].

We investigate and compare the changes in morphology and the electro-optical behaviour of thin film organic solar cells, utilising low cost polymers such as PTQ10 and non-fullerene acceptors such as BTP-4F, processed from various solvents, utilising grazing-incidence X-ray scattering methods, time-resolved transient absorption spectroscopy, and nanoscale FTIR. We show the impact of solvent composition on the formation of polymer:non-fullerene acceptor bulk heterojunction films, affecting the resulting change in the performance of the organic solar cells. This leads us to a better understanding on the way to developing high efficiency, environmentally friendly, flexible solar cells.

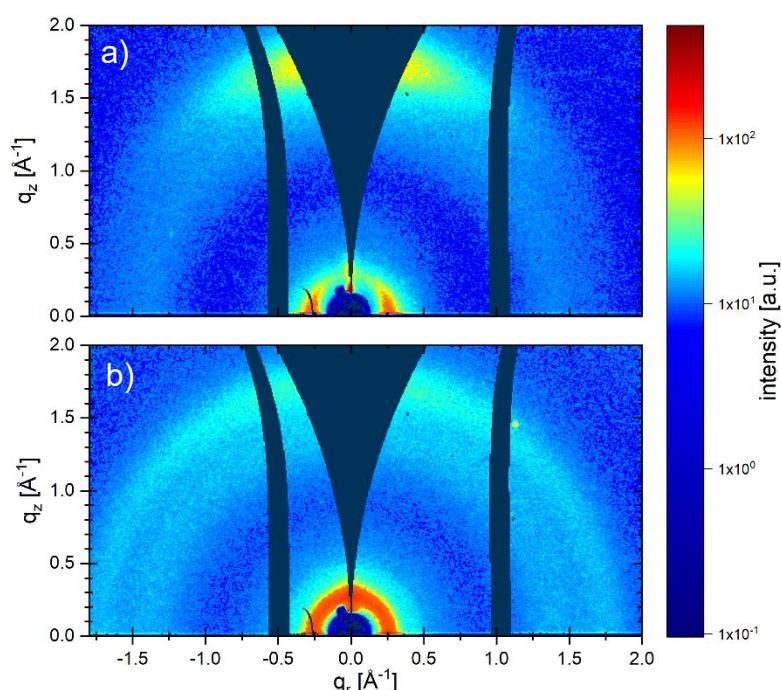


Figure 1: Grazing incidence wide-angle x-ray scattering images of PTQ10:BTP-4F bulk-heterojunctions produced from a) chloroform, b) 1,2,4-trimethylbenzene

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Dynamics in polymer-fullerene blends for photovoltaic applications

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In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed and excitons are created. After diffusion to a donor-acceptor interface, the excitons are dissipated and charge carriers can be extracted from the electrodes.

From the early years of organic photovoltaics on, the combination of P3HT ((C₁₀H₁₄S)_n) as electron donor and PCBM (C₇₂H₁₄O₂) as electron acceptor is a frequently applied and well-studied system. Previous studies have shown that both, internal dynamics and structural layout of the active layer influence electronic properties and thus also performance of a device.

A more modern, very promising low-band gap electron donor material is PTB7 ((C₄₁H₅₃FO₄S₄)_n).

Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, PCBM and different blends of these two, prepared out of chlorobenzene solutions, and performed first quasielastic neutron scattering experiments at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching).

Hydrogen dynamics of pure compounds as well as the blend films are investigated on a pico- to

nanosecond timescale in a temperature range from 150 K to 400 K. E.g. diffusion coefficients are calculated for the respective samples, as suggested by Figure 1. Results are set into context of photovoltaic performance studies and increase the knowledge base, which is needed for the design of new materials to push the field of organic photovoltaics.

Figure 1: Diffusion coefficients for pure PTB7 and two PTB7:PCBM blends, determined with quasielastic neutron scattering. Polymer:fullerene ratios are based on weight.

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.

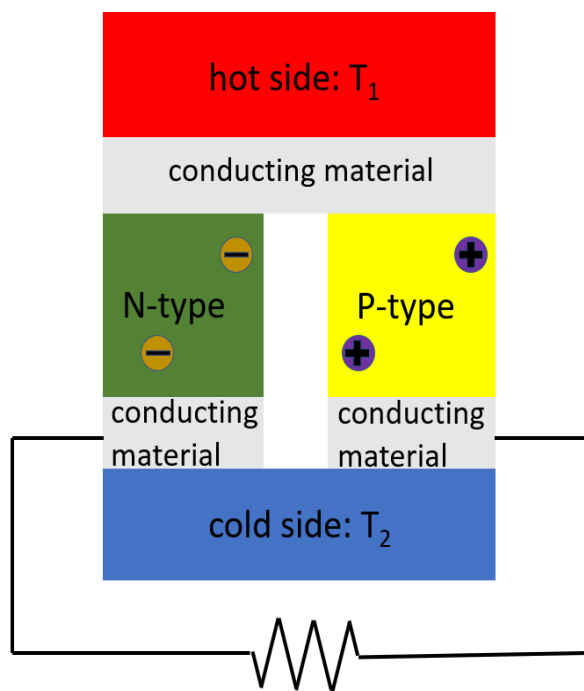


Figure 1: Thermoelectric circuit composed of an n-doped and a p-doped material. (different Seebeck coefficients)

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 bio-polymer, that is known to form different aggregates under different environmental conditions. At low ph-values (ph = 2) it can form fibril structures, while close to the isoelectric point (ph~4.2) it forms globular structures. Therefore, beta-lactoglobulin is used to structure Titania (TiO_2) using Sol-Gel synthesis with water as the solvent. Spray coating is used to enable industrial mass-production. A big focus is on the use of non-toxic and abundant materials.

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, thermal conductivity 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.

Identification of intra wind farm flow

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Wind farm control applications require an accurate prediction of turbine wake impingements. While low-cost engineering wake models have been greatly improved over the years, the embedding farm background flow is often assumed homogeneous, which is hardly true. This contribution will present methods to detect long- and short-term heterogeneities in the ambient flow from turbine production data.

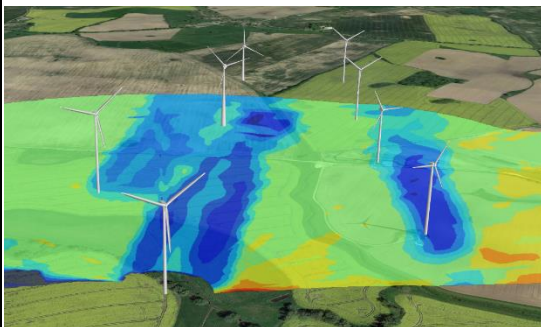


Figure 1 Wind farm flow measured by a LIDAR

Inside a wind farm, the long-term heterogeneous flow field will be caused by the permanent presence of orography, obstacles and surface roughness. Even for offshore farms, the influence of land can still inflict persistent gradients in the array inflow wind speed [1]. A further source for flow heterogeneities can be the wind farm itself by interacting with the atmospheric boundary layer, often divided in blockage and deep array effects. As was presented in [2], a baseline engineering model like Floris [3], can be adapted to a specific site by infusing and learning parametric correction terms. The observational data, that is used for this tuning, is

ordinary SCADA data from the turbines themselves. A heterogeneous flow field can then be detected by identifying flow tuning nodes. The site specific wake model parameters are simultaneously tuned. This rather ill-conditioned optimization problem is solved by mapping the tuning parameters into an orthogonal space via singular value decomposition (SVD), which leads to robust convergence.

Figure 2 shows the identified flow field for the Italian wind farm Sedinì. The locations of flow tuning nodes are marked with "x". It is visible, that the wind speed was adapted in different regions of the farm. These corrections can be validated with a CFD RANS simulation, that models the surrounding terrain. First results of an OpenFOAM simulation show, that the identified corrections are indeed in the right order of magnitude.

The second research goal presented is to apply the correction methodology on shorter time scales to identify dynamic flow heterogeneities. As turbine array sizes increase, changes in wind speed and direction cannot be assumed to affect all turbines instantaneously. Rather, ambient conditions propagate through the array, which can be shown for the Anholt wind farm. Together with a propagation model, the identification methodology can be used "on the fly" to detect local wind speeds and directions.

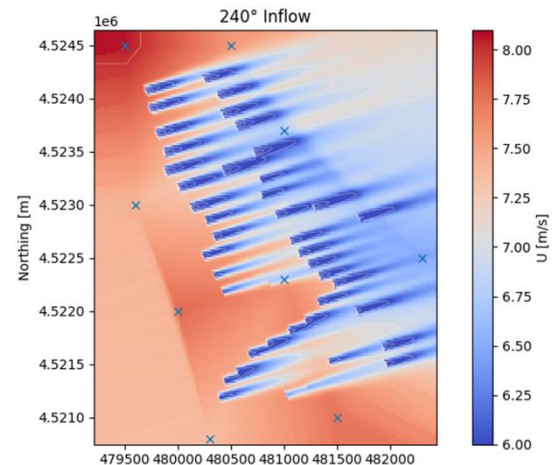


Figure 2 Wind farm simulation with heterogeneous background flow

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In Operando Studies of Solid Polymer Electrolyte for Thin Film Lithium Ion Battery

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Lithium ion batteries (LIBs) emerged as the most promising candidate for electrochemical energy storage owing to its higher specific energies, volumetric energy densities and power densities with a wide range of applications, ranging from digital cameras to pure-electric vehicles. Solid polymer electrolyte (SPE) is attractive for the next generation batteries regarding its thermal stability comparing to the liquid electrolyte and simpler manufacturing than ceramic-based electrolyte.¹ PEO-based electrolyte, as the most widely used SPE, however, is facing significant challenges due to its narrow electrochemical window and the interface instability above 4 V vs Li⁺/Li, meaning that such SPE is more instable in high-energy-density batteries.^{2, 3} In order to alleviate this hinderance, the 1,2-dimethoxyethane (DME) was introduced to PEO/ lithium bis(trifluoromethanesulfonyl)imide (LiTFSI) electrolyte. A series of Li(DME)_xTFSI-PEO_y (x= 0.6-1.2, y= 0.5-1.0) electrolyte was prepared and LiTFSI-PEO_y electrolyte as comparison. Li||Cu cell and Li||NMC₃₃₃ cell are fabricated to evaluate the electrochemical properties of electrolyte. The nanoscale morphology and structure of the electrolyte after certain plating/stripping cyclings are investigated via in operando Small-angle X-ray Scattering (SAXS).

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Integrated Capture and Conversion of CO₂ to Methanol

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Efficient carbon capture and utilization (CCU) is a key process for a sustainable methanol economy. This requires integrated processes, where CO₂ is captured as well as converted by the same material, with the possibility to operate under dynamic reaction conditions in order to provide the required flexibility for the fluctuating and non-stationary energy demand. Methanol, in turn can be used as an energy carrier, that can be either combusted directly in conventional engines or used as a hydrogen carrier for methanol fuel cells. Additionally, methanol can be used as a C1 building block for a variety of products.

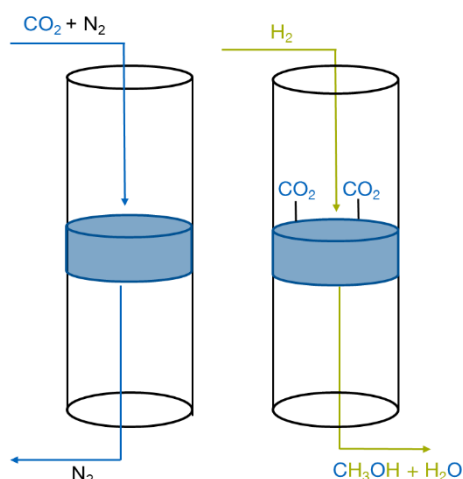


Figure 1: Basic concept of integrated CCU.

The silica based catalyst was prepared by a sol – gel based synthesis method yielding mm sized silica spheres, which were functionalized with 3-aminopropyl-triethoxysilane and Palladium particles. The catalytic activity was measured in a fixed bed reactor at 1 bar pressure during dynamic changes in the reactant feed (10% CO₂/He at 70 °C followed by hydrogenation with 78% H₂/He up to 140 °C). Operando IR-spectroscopy was used to analyze the surface species present during CO₂ adsorption and the subsequent hydrogenation of adsorbed CO₂ to methanol.

A CO₂ conversion to methanol of up to 25 % (0.01 CH₃OH mol/mol NH₂ groups) based on the irreversibly CO₂ adsorption capacity, with a selectivity of 100 % towards methanol and water was observed (see Fig. 2). CO and CH₄ formation was not observed in any of the experiments. Catalysts loaded with amine or Pd only did not show any conversion of CO₂ to methanol.

In the bifunctional catalyst, the amines (NH₂) serve as site for binding and activating the CO₂ and the Pd activates H₂ for the hydrogenation of the bound CO₂ to methanol.

Using IR – spectroscopy, we were able to identify the reaction intermediates and together with the finding, that the amine – Pd interface constitutes the active site for the conversion, we are now able to further improve the performance of the catalyst.

In this presentation we discuss the development of a novel concept for integrated CCU based on a new type of bifunctional catalysts that are able to capture and selectively convert CO₂ to Methanol under dynamic and mild reaction conditions (140 °C, 1 bar).

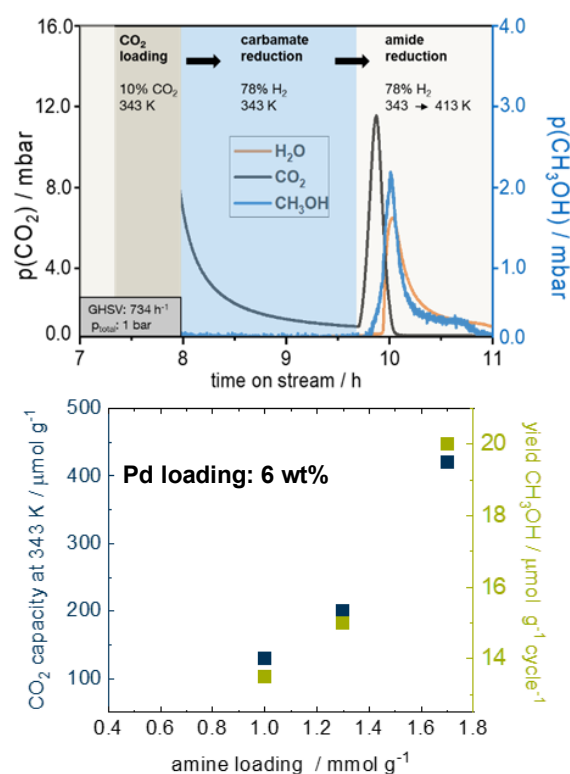


Figure 2: (top) reaction sequence of the dynamic reaction operation; (bottom) methanol yield as function of metal – amine interface.

Integrating Building Performance Simulation Results and Boundaries in IFC (Industry Foundation Classes)

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Nowadays, in the Architectural, Engineering and Construction (AEC) industry, Building Information Modelling (BIM) is gaining momentum in its practice and usage. BIM optimizes the work of construction engineers, saves time and costs, opens new horizons in communications and coordination. Various BIM software solutions provide tools for designing, structural analyzing, and Building Performance Simulations (BPS). Many of these software uses an open object-oriented file format called Industry Foundation Classes (IFC). IFC is vendor-neutral, and it facilitates the information exchange process during the whole life cycle of construction and maintenance.

Regarding BPS software, the development of the Building Energy Model (BEM) stays apart from architectural BIM in many cases and implies the work of an energy engineer in the preliminary design stage (Figure 1). Some BPS software support import of IFC files (e.g., Autodesk Inc (2020), Graphisoft SE (2020)), but very few of them can preserve the results and integrate them into the IFC files. After setting boundary conditions and getting simulation results, the data is exported in a specific format but generally not exported to the IFC

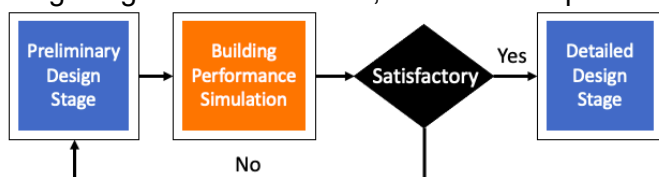


Figure 1: BPS in the Preliminary design stage

format for further proceeding. The integration of BPS results in the original designed model and exporting them to a complete and consistent IFC file could help to improve the collaborative workflow between the project participants. It could expand the IFC format's functionality and preserve the comprehensive design information for future reuse.

This research will investigate possible ways of integrating BPS simulation data and boundary conditions in the IFC file and provide a proof of concept for that. Regarding the integration approach, the corresponding ontology will be developed and tested with a developed software prototype (Figure 2). The results will be compared with existing approaches. The occurred problems will be analyzed. The findings should provide theoretical knowledge and practical steps in facilitating BIM and BEM data exchange for all the involved specialists: architects, engineers, energy efficiency consultants, etc.

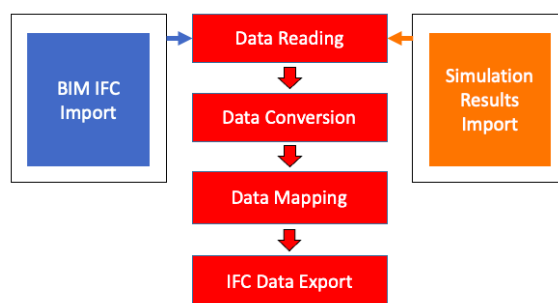


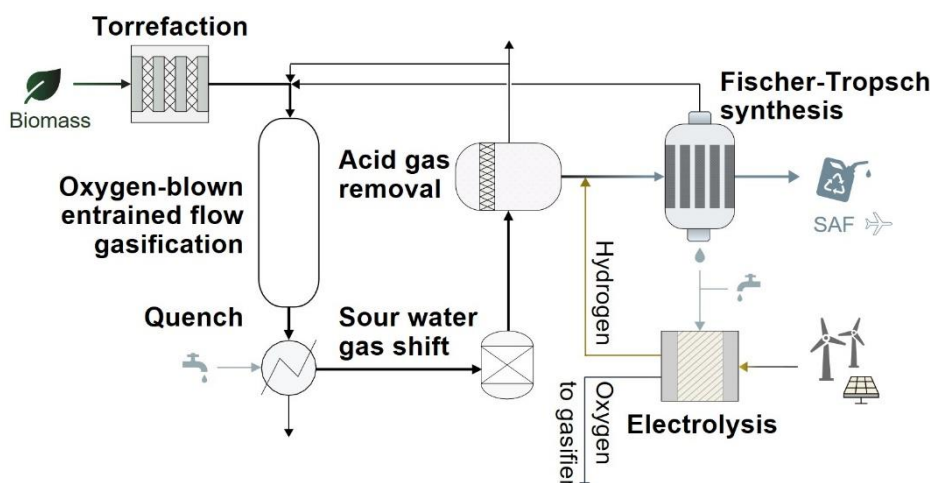
Figure 2: Concept scheme for data processing in the software prototype

Using Hydrogen and Oxygen from Electrolysis to Improve Carbon Efficiency for an Advanced Biomass-to-Liquid Process producing SAFs

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Long-distance transportation, especially aviation, will continue to depend on energy sources with high energy density. To end the dependence on fossil fuels and mitigate the expected global growth of air traffic in the coming decades, the only realistic strategy for GHG reduction in aviation are alternative "drop-in" fuels. For such sustainable aviation fuels (SAF) to have a positive impact, energy sources such as biomass residues or renewable electricity must be utilized. The thermochemical biomass-to-liquid (BtL) conversion route, which uses lignocellulosic biomass such as carbon-neutral biomass residues as feedstock, is considered one of the most promising alternative pathways for producing bio-based drop-in fuels. However, BtL processes typically result in low system performance because the carbon efficiency of the overall process is limited.



A novel approach, combining electrolysis and oxygen-blown entrained flow gasification enables high carbon efficiency for producing sustainable Fischer-Tropsch fuels. The combination of using biomass as the carbon and energy source and hydrogen as an energy carrier supplied from carbon-neutral renewable energies makes it possible to overcome the carbon efficiency limitation of conventional BtL processes. The special feature of this approach is the complete utilization of the electrolysis

Figure 2: Simplified schematic (P)BtL process flowsheet producing SAFs

products as hydrogen integration in biomass-based processes allows the oxygen produced during electrolysis to be used for biomass gasification. Hybrid Power-and-Biomass-to-Liquid (PBtL) systems thus enable higher carbon efficiency than conventional BtL concepts at lower hydrogen requirements than pure PtL alternatives.

At the Chair of Energy Systems of the Technical University of Munich (TUM), a highly integrated BtL process is modeled using the process simulation software Aspen Plus[®] to identify the optimal solution in terms of energy and material efficiency. The model is designed so that the associated subsystems can be plugged into its hierarchical framework. The model consists of pretreatment via torrefaction of lignocellulosic biomass feedstock, syngas generation through oxygen-blown entrained flow gasification, partial quenching and hot solids and halides removal, sour water gas shift (WGS) to adjust the H₂/CO ratio, acid gas removal using adsorption technologies at elevated temperatures, and FT synthesis to produce SAFs.

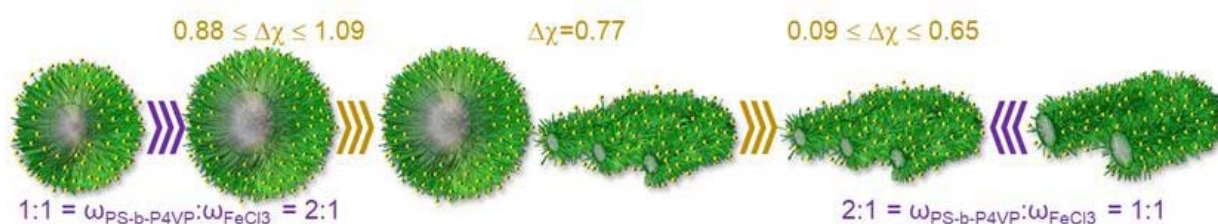
To enhance process performance, integrating green hydrogen and oxygen from water electrolysis is modeled and the use of polymer electrolyte membrane and solid oxide electrolysis at elevated temperature is compared. To investigate the potential of the hybrid approach, the process configurations where hydrogen is added to the FTS reactor to reach the desired H₂/CO ratio are simulated with increasing electrolysis size up to a maximum in carbon efficiency of 97%. By adding hydrogen from electrolysis, the product yield is increased by a factor of 1.7-2.4.

Morphology control of PS-*b*-P₄VP templated monolayer mesoporous Fe₂O₃ thin films

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Mesoporous Fe₂O₃ thin films with large area homogeneity demonstrate tremendous application potential in photovoltaic industry, lithium ion batteries, gas or magnetic sensors. In the present work, the synthesis of morphology - controlled Fe₂O₃ thin films is realized with the polystyrene-block-poly(4-vinylpyridine) (PS-*b*-P₄VP) diblock copolymer assisted sol-gel chemistry. The effect of the solvent category and polymer-to-FeCl₃ ratio is systematically investigated during the sol-gel synthesis process. Spin coating is used for the thin film deposition and an calcination process in the air condition is used for removing the PS-*b*-P₄VP polymer template. For both DMF and 1,4-dioxane solvent system, nanocluster structures are obtained with low PS-*b*-P₄VP concentration, which is supposed to be the result of the weak phase separation property and thereby the weak template effect of the block polymer. When the concentration of the PS-*b*-P₄VP reaches the critical point of micellization, spherical and wormlike porous structures can be specifically formed in the DMF and 1,4-dioxane solvent system, respectively. The further increase of the polymer-to-FeCl₃ ratio lead to the enlargement of the spherical pore size in the DMF system and the shrink of center-to-center distance of the worm like structure in the 1,4-dioxane system. Moreover, DMF/1,4-dioxane solvent mixture with different volume ratios are applied for the sol-gel solution preparation to trace the effect of the solvent selectivity on the thin film morphology. By adjusting the preferential affinity of the solvent mixture to the polymer blocks, a spherical to wormlike pore shape transition is observed near a critical $\Delta\chi$ value of 0.77.



Spray-deposited anisotropic ferromagnetic hybrid polymers films of PS-*b*-PMMA and strontium hexaferrite magnetic nanoplatelets

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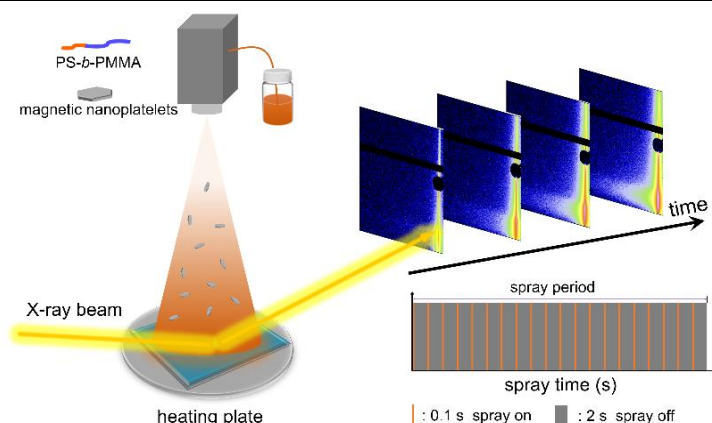


Figure 1: Schematic of the spray deposition with simultaneous in situ GISAXS measurements

Magnetic nanoparticles (NPs) have gained increasing research attention for a broad range of applications that include magnetic sensors, catalysis, magnetic energy and data storages. In some applications, precise control over their arrangement is essentially required. Diblock copolymers (DBC)s have proven to be suitable templates for hosting iron oxide NPs, due to their ability to form various periodic nanostructures, such as spheres, cylinders, and lamellae.

In this work, M-type hexaferrite magnetic nanoplatelets with a platelet-like shape and a high magnetic anisotropy are used as magnetic NPs. Spray deposition, a scalable technique, is applied to fabricate anisotropic ferromagnetic hybrid polymer films by controlling the orientation of strontium hexaferrite nanoplatelets inside ultrahigh molecular weight DBC polystyrene-*block*-poly(methyl methacrylate) (PS-*b*-PMMA) films. During spray deposition, the kinetics of structure evolution of the hybrid film are monitored in situ with grazing-incidence small-angle X-ray scattering (Figure 1). The obtained final dried films are then solvent annealed inside a closed chamber with tetrahydrofuran (THF) to study the influence of solvent vapor annealing (SVA). To probe the surface structures and magnetic properties of the final films before and after SVA, characterizations, with scanning electron microscopy (SEM) and superconducting quantum interference device (SQUID) magnetometry, are applied. Due to the rearrangement of the nanoplatelets inside the DBC during SVA, obvious changes in the morphology and magnetic behavior of the hybrid film are observed via SEM and SQUID, respectively.

The scattering data suggest that the magnetic nanoplatelets are tilted with the large facet close to the substrate surface for the hybrid system. A decrease in the average tilt angle between the nanoplatelet large facet and substrate surface normal is observed over time. SQUID investigation indicates that ferromagnetic hybrid polymer films with high coercivity can be achieved via spray deposition, which is beneficial to scale up the fabrication of hybrid films for magnetic data storage applications. Moreover, the hybrid film shows perpendicular magnetic anisotropy before SVA while a weak magnetic anisotropy remains after SVA (Figure 2), which renders these hybrid films appear highly promising for potential applications in magnetic sensors and data storages.

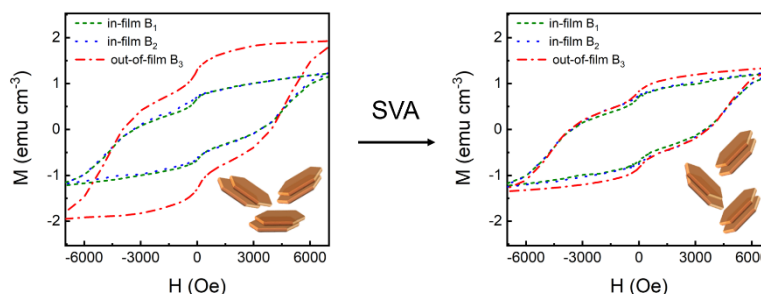


Figure 2: Magnetic properties before (left) and after (right) SVA

OSkit – Optimized Sector Coupling in Districts through Intelligent Thermal Prosumer Networks

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The change from a fossil to a renewable-dominated energy system has to include the three essential sectors electricity, heat, and transport. The coupling of the electricity and heat sectors is an effective and cost-efficient tool to compensate for fluctuations of volatile, renewable electricity generators and to reduce the load on the distribution grid.

Current approaches in sector coupling of electricity and heat mostly follow a strict decentralized or centralized approach for heat supply. In OSkit, on the other hand, the advantages of centralized and decentralized heat supply are to be combined into a prosumer-based, flexible and bidirectional heat network. The optimized decentralized heat supply preserves the advantages of the decentralized energy supply, but makes better use of the devices, like CHPs, heat pumps, or solar thermal collectors in the network and exploits the potential for sector coupling to a greater extent.

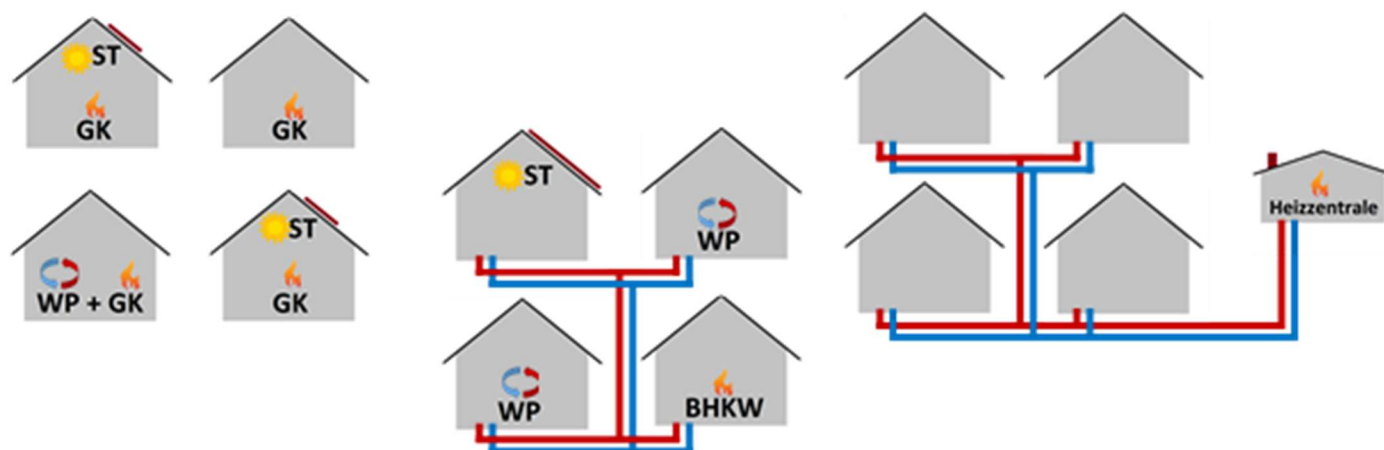


Figure 1: Conventional decentralized (left) and centralized (right) approaches to heat supply are combined to form a prosumer-based heat network (center).

The project will develop and analyze new, innovative topologies for thermal grids and their bidirectional transfer stations. This will require suitable central and decentral operating strategies for the transfer stations and the operation of the thermal and electrical systems. The novel thermal and electrical microgrid will then be validated in the CoSES laboratory and the potential impact on the distribution grid will be analyzed. In addition, techno-economic implementation options will be investigated in a field test.

Uncovering the enhancement mechanisms of thermoelectric performance of PEDOT: PSS films after physical-chemical dedoping

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Organic semiconductors have attracted intense attention because of their potential use in mechanically flexible, lightweight, and inexpensive electronic devices. Especially, poly(3,4-ethylenedioxy thiophene): 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 in thermoelectric (TE) devices [1,2]. The energy conversion efficiency of a TE material is evaluated by a dimensionless figure of merit ZT and defined as $ZT = S^2\sigma T/k$ where S is the Seebeck coefficient, σ is the electrical conductivity, T is the absolute temperature, k is the thermal conductivity, and $S^2\sigma$ is defined as the power factor (PF) [3,4]. Nevertheless, it is generally acknowledged that it is difficult to achieve a high ZT value of TE materials, due to the fact that the parameters S , σ , and k are interdependent as a function of the carrier concentration and hard to be optimized simultaneously. In this work, we adopt a combination of DMSO addition and subsequent DMSO post-treatment to engineer TE performance of PEDOT:PSS thin films. Results show that the as-obtained PEDOT:PSS film presents a maximum PF of $64.4\mu\text{W}(\text{m}\cdot\text{K}^{-2})$, which is a ~ 1073 -fold leap larger than that of pristine film. The origin and mechanism of the underlying improvement are systematically investigated by various characterization techniques to gain a more profound understanding of the fundamental nature of the modified PEDOT:PSS films.

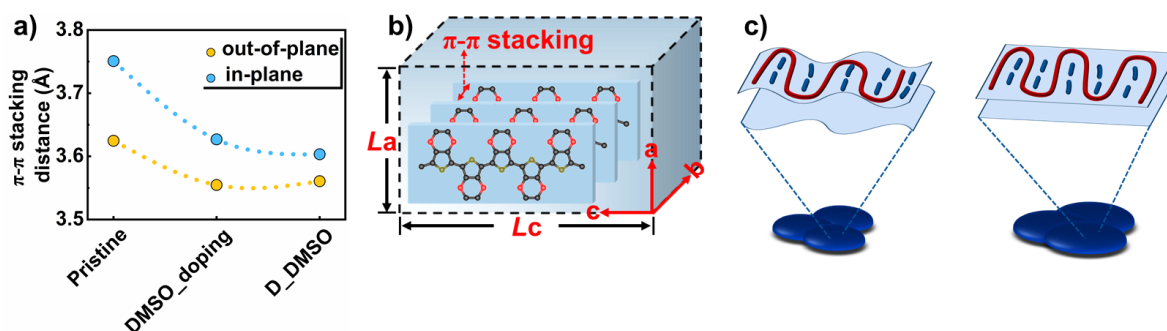


Figure 1: a) π - π stacking distance, b) crystalline domain in PEDOT:PSS films, c) schematic diagrams showing the structural change of the PEDOT:PSS films.

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Measurement setup to characterize thermoelectric polymer thin films

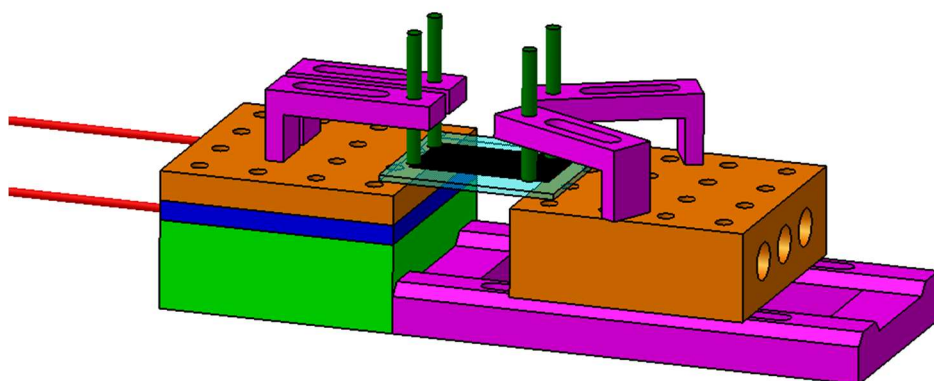
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The growing need to save fossil resources requires besides their substitution also the effective usage of these. This usage is mostly limited by the high amounts of wasted heat in the conversion from chemical energy to mechanical or electrical energy. The most known example is the combustion engine. Even modern diesel have a thermal efficiency of less than 50%. [1]

Thermoelectric (TE) materials are a promising way to make use of this wasted energy. Particularly, they can be used in a wide range of applications to generate electricity. Nevertheless, these materials show lots of room for improvement in terms of their output power. To enable research on this it is important to have the opportunity to rapidly characterize a big number of potential TE materials. Therefore, with our work, we aim to construct a setup, which focuses especially on the measurement of polymer-based TE materials for low-temperature applications. This setup consists of two mounting plates that can be heated or cooled individually to determine the Seebeck coefficient at different temperatures. Additionally, a van der Pauw measurement can be done to find the electrical conductivity of the sample. By this, the setup will enable the user to characterize the sample by its TE power factor, which describes the outputted electrical power in terms of the applied temperature difference.

Further requirements of the future measurement setup are, that it is supposed to be as modular as possible, allowing the adjustment to different sample sizes and sensors. Besides, it should be possible to do scattering experiments with neutrons or X-ray techniques, while the thermoelectric material is in operation. For this, the whole setup is planned to be included in a special vacuum chamber.



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Estimating onshore wind experience curves for energy system models – a multi-factor approach

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Estimated onshore wind learning rates span a large range of about 40 percentage points. This uncertainty is particularly problematic for forward-looking energy system models that depend on precise point estimates to accurately model future power system costs.

We propose a multi-factor experience curve model with a new economies-of-scale measure and estimate it using country-level data from seven European countries. We find learning by doing rates of 2% - 3% and learning by searching rates of 7% - 9% in terms of LCOE but no significant learning in onshore wind installed costs. Further analysis reveals that learning, particularly learning by searching, can be found when approximating technological change with the capacity factor rather than costs. Hence, energy models that endogenize technological change should also implement learning rates for capacity factors and operational expenses in order to grasp all technological progress materializing in onshore wind. We also investigate several potential drivers of sensitivity in learning rates. Besides the definition of the cost measure, the measurement of the knowledge stock and its assumed depreciation rates have large effects on learning rates in our sample.

Mesoporous ZnO thin films templated by diblock copolymer for photovoltaic applications

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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.

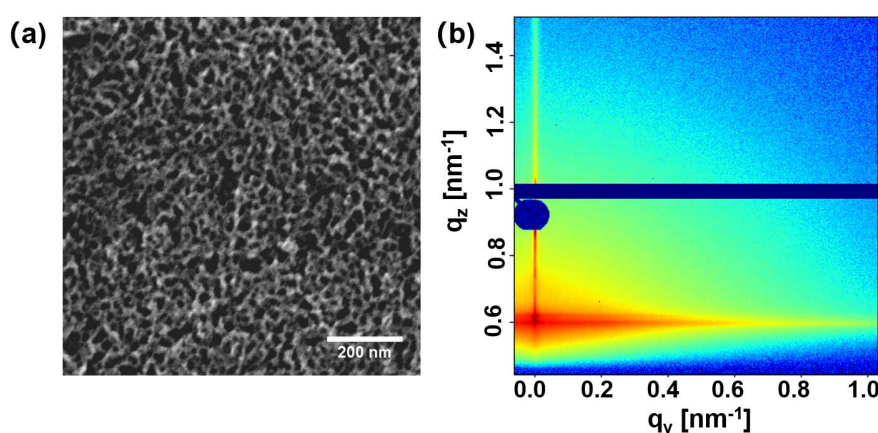


Figure 1: a) SEM images and b) 2D GISAXS data of printed mesoporous ZnO films after template removal.

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Understanding the Chemistry of Alcohol Photocatalysis for Sustainable Hydrogen Production

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Associated with the worldwide population growth, energy consumption rapidly increases. In order to reduce concomitant greenhouse gas emissions and meet the challenges of climate change, it is crucial to find sustainable energy sources. In this regard, hydrogen as a zero-carbon emission energy carrier with a high specific energy content has increasingly gained attention. However, to avoid fossil fuel consumption and CO₂ emission from steam reforming, which is the most common way to produce hydrogen until now, an alternative method utilizing renewable feedstocks must be developed.

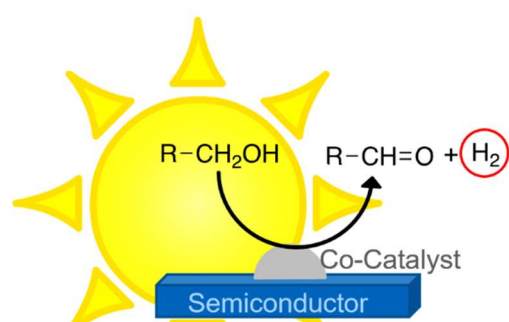


Figure 1: Photocatalytic alcohol conversion on a co-catalyst loaded semiconductor support.

In this respect photocatalysis is a promising research field, aiming to generate hydrogen from water or biomass-derived alcohols by harvesting solar light.^[1] In heterogeneous photocatalysis the catalysts are usually based on semiconductors. Just as in a solar cell, light absorption leads to charge carrier formation in the bulk material. These charge carriers diffuse to the surface where they can induce chemical reactions. This way, the energy of the photons is converted to chemical energy, with the most prominent example being the formation of molecular hydrogen (H₂).^[2]

In the past 30 years, numerous photocatalytic experiments were carried out on noble metal-loaded, powdered semiconductors under ambient conditions.^[3,4] However, the complexity and large variety of the photocatalysts explored in those studies precludes a deeper understanding of the general principles of the system. The investigation of photocatalytic processes under highly defined conditions, i.e. under ultra-high-vacuum (UHV) on atomically defined semiconductor single crystals, allows to link distinct material properties to the catalysts' performance, and hence facilitates insights into fundamental mechanisms.

In our experiments, alcohols are investigated as model substrates for photocatalytic reactions, since they are hydrogen carriers and biomass derivatives. The deposition of small metal particles ("clusters") onto the semiconductor surface was found to be necessary for enabling hydrogen evolution from photocatalytic alcohol reforming in UHV.^[5] Herein, we elucidate the individual contributions of the semiconductor and the metal cluster co-catalysts in such systems. In-depth investigations about the effect of different cluster sizes and coverages on the photocatalytic activity are shown in the contribution "Material Design Parameters for the Generation of Hydrogen on Semiconductors from Light". Our approach allows targeting well-defined systems for future catalytic applications.

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Life Cycle Assessment of vertical building extensions in early design stages

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Figure 1: Visualization on the Collaborative Design Platform (CDP)

Densification is a common way to create additional living space in urban areas. Through their connection with the existing building stock, building extensions have to be designed carefully to achieve good performance in climate change adaption and mitigation. Within the research project “Densification in context of climate change” we assess these environmental impacts by using the Collaborative Design Platform (CDP), which was developed at the chair of Architectural Informatics at TUM [1]. Through that, building geometry based on Open Street Map (OSM) data can be extracted and modified, with results visualized in real-time. One common type of densification is the vertical building extension. As there is only little semantic information available regarding the urban building stock, a methodology for Life Cycle Assessment (LCA) calculation has to be developed for this few information.

To assess the environmental impact of a vertical extension, the scope for LCA is separated into three parts. First, the demolished components are calculated by extracting roof area and building age class from the 3D model. Through the combination with the typical constructions retrieved from the TABULA project [2], the environmental impact per square meter is calculated. Depending on the roof type (either flat or pitched) a literature-based reinforcement structure is chosen. These structures are modeled in the eLCA Software [3] and exported in CSV file format. The new building parts are also modeled in eLCA based on different sources, e.g. dataholz.eu or literature. The CDP user can either choose a specific construction or get a range of possible values. Finally, the sum of environmental impacts of demolished, reinforced, and newly built structures is calculated and displayed on the CDP user interface. As the connection between the mentioned software, databases, and the CDP, Python programming language is used.

In the next step, the described methodology will be implemented to CDP. This will allow real-time feedback on grey emissions for vertical building extensions. In parallel, we are working on a methodology for real-time assessment of energy consumption of extended buildings. The combination of both will allow users to evaluate vertical building extensions scenarios in the early design stage regarding their lifecycle impact.

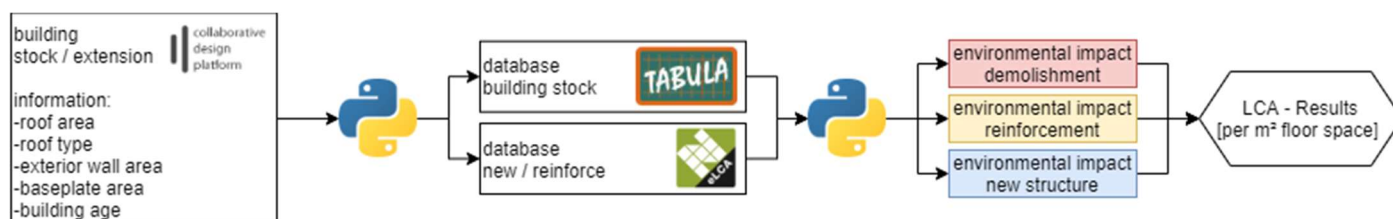


Figure 2: Methodology to assess LCA of vertical building extensions from CDP information

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The research project ‘Densification in context of climate change’ is funded by Bavarian State Ministry of the Environment and Consumer Protection (StMUV) and the TUM Centre for Urban Ecology and Climate Adaption (ZSK).



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Slot-Die Coating of Perovskite Solar Cells: A Technique for Upscaling

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Perovskite solar cells (PSCs) have attracted increasing attention in research and industry due to their high efficiency, low material cost, and simple solution-based fabrication process. In laboratory devices, the efficiencies are already comparable with c-Si and thin-film technologies. In the recent past, most of the work focused on increasing the performance and the stability of perovskite devices, achieving encouraging results: the PCE increased from 3.8% to more than 25% in 10 years. ^{[1][2]} However, towards commercialization, one of the technologically most important steps is upscaling of PSCs to a larger area.

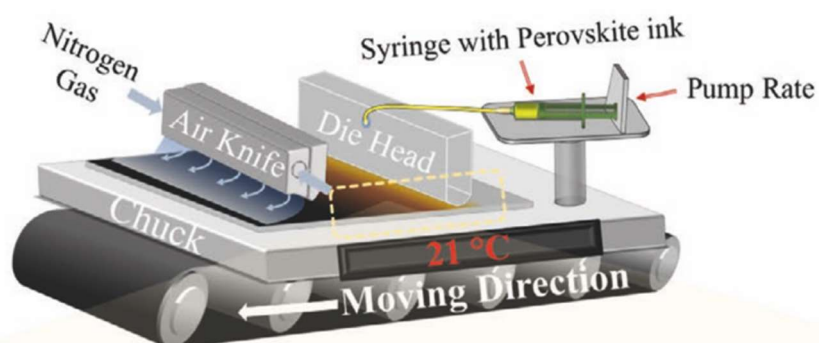


Figure 1: Slot-die coating apparatus. [3]

Slot-die coating is considered to be one of the most promising technology to produce commercial-size perovskite solar cells, being a fast process with minimum material consumption and waste. ^[4] Furthermore, the highly tuneable perovskite ink composition strongly determines the final morphology of the film, providing an outstanding opportunity to develop a comprehensive understanding of the kinetic processes during film formation. The main focus of our work is to investigate suitable ink compositions and the resulting final perovskite thin-film with spectroscopic and X-ray scattering methods to develop a standardized reproducible technique for printed flexible and high-efficiency PSCs.

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In situ GIXS observation of spray coating lead-free perovskite on mesoporous titania

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Perovskite solar cells are very promising candidates for both, highly efficient and economically fabricated photovoltaics, because of their optoelectronic characteristics and solution processibility. Most of the current research focuses on lead-based systems. Despite their outstanding performance, lead-based perovskites show comparatively low stability at ambient atmospheric conditions. Besides this, the involved water-soluble lead compounds and toxic organic solvents limit the environmental friendliness of these auspicious photovoltaic systems, especially when fabricated on an industrial scale. In order to overcome this challenge, we are interested in the fabrication of perovskite systems of reduced toxicity. For this, we investigate a lead-free perovskite based on methylamine, bismuth, and iodine (MBI). Bismuth is more stable against oxidation compared to other lead-free, tin-based perovskites, while having a similarly polarizable electron density as lead. By mixing methylammonium iodide and bismuth iodide with the non-toxic solvent methyl-acetate, an MBI perovskite solution is obtained [1]. This solution can then be processed by large-scale deposition techniques like spray or slot-die coating at ambient conditions.

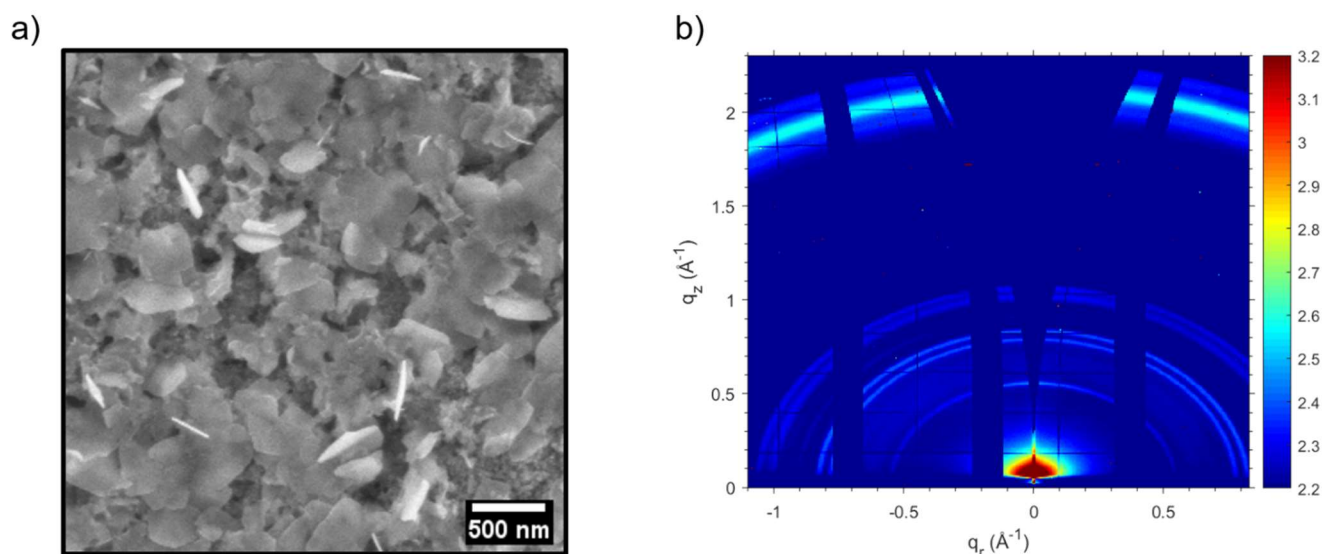


Figure 1: MBI perovskite on mesoporous titania after spray coating. a) scanning electron microscope image b) GISAXS/GIWAXS detector image

In this work, we investigate the film formation and crystallization of MBI on mesoporous titania during spray coating by simultaneously measured in situ grazing-incidence small-angle and wide-angle X-ray scattering (GISAXS/GIWAXS) in real-time. GISAXS/GIWAXS measurements are complemented with real-space imaging, such as optical and scanning electron microscopy. From these insights, further research on improving stability and performance of lead-free perovskite systems can highly benefit. Furthermore, the mesoporous titania substrates were fabricated by a water-based, low-temperature route to promote the green character of the perovskite fabrication.

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Open database system for the collection, management, and strategic analysis of heterogeneous data sets of large building portfolios

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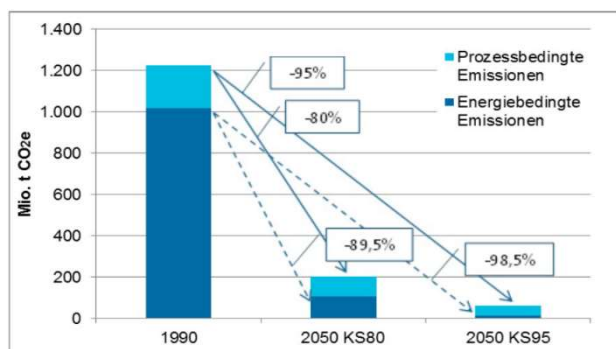


Figure 1: Development of GHG emissions of the nationwide climate protection scenarios, which serves as the basis for the scenarios calculated for Munich. [1]

RESEARCH APPROACH

The Paris Climate Agreement of December 12, 2015 is an important milestone in the fight against global warming. With its Climate Protection Plan 2050, the German government has set itself the goal of becoming largely greenhouse gas neutral by 2050. Currently, around a quarter of all CO₂ emissions are attributable to the building sector. The potential for savings is therefore huge. To meet the targets, greenhouse gas emissions in the building sector must fall by 66 to 67 percent by 2030 compared with 1990 levels [2].

Managers of large building portfolios can make a significant contribution to achieving the targets through smart retrofit management. Large amounts of data, from various sources, with often insufficient building information, pose a major challenge to portfolio managers. In this context, the research project "OfDataLyse" aims to produce a transferable methodology for energy-related building portfolio management, using the example of the City of Munich. In the process, an intelligent database system will be developed that enables the collection, management, and analysis of complex building data.

OBJECTIVES

In the sense of strategic portfolio management, the aim is to use the existing data of the city of Munich to obtain a comprehensive assessment of the energy status of the buildings and to identify the renovation measures and their effects.

METHOD

The data stock of the state capital Munich serves as a basis. First, all relevant parameters are collected in a database. The master data are supplemented with further parameters, for example with data from geoinformation systems. Statistical values also contribute to the expansion and closing of data gaps. Regression analyses will be used to make data correlations recognizable (Figure 2). The knowledge gained should help to identify relevant building parameters. Depending on the data basis, the renovation and savings potentials of the buildings are determined using appropriate calculation algorithms.

PROSPECTS

The method will be applied and tested on the building stock of the city of Munich.

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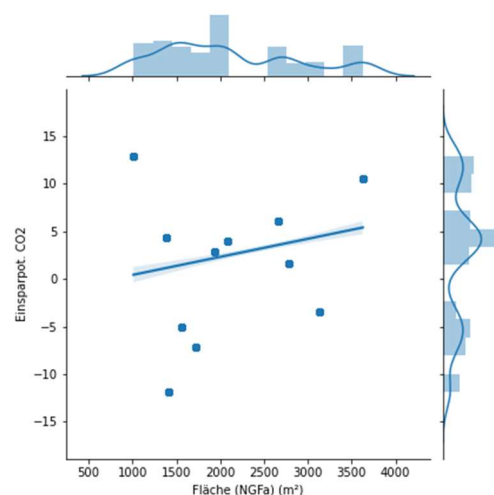


Figure 2: Correlation between CO₂ savings potential and net floor area

Optimal feedforward torque control for doubly-fed induction generators in wind energy conversion

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Motivation

Doubly-fed induction generators (DFIGs) with grid-connected stator and inverter-fed rotor are widely used in wind energy conversion systems [1]. The objective of optimal feedforward torque control (OFTC) is to provide the reference torque while minimizing losses. Thus, an optimal reference current computation (ORCC) is desirable which minimizes the current-dependent DFIG losses while reaching the reference torque and taking into account operating (e.g. current & voltage) limits. Existing approaches are either based on simplified modeling or LUT-based approaches using numerical calculations or expensive measurements. The proposed method is based on an advanced DFIG model and allows for *analytical* ORCC taking into account (i) *nonlinear magnetic saturation*, (ii) *cross-coupling effects*, and (iii) stator *and* rotor copper losses.

Methodology

The magnetic flux linkage maps (cf. Fig. 1), obtained by measurements [2] or finite element analysis (FEA), are linearized at the actual operating point such that the idea of *sequential quadratic programming* is applicable which consists of three main stages per sequence: (i) *quadratic approximation* of the constrained nonlinear optimization problem, (ii) applying the *Lagrangian* formalism to solve the quadratic (sub-)problems (QPs), (iii) selection of the optimal solution [3]. It can be shown that the solution of the QPs is given by the intersection point of two *quadratics*, which can be calculated analytically [4]. Based on the current loci in Fig. 2 an *operation management* was designed which saturates the torque and chooses the optimal operating strategy, namely *Maximum Torque per (copper) Losses* (MTPL_{cu}) or *Maximum (rotor) Current* (MC_{r,ext}).

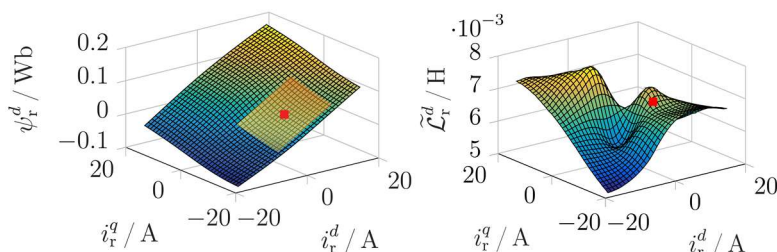


Fig. 1 Rotor d-flux linkage (left) and partial derivative with respect to the rotor d-current (right).

Results

The OFTC accurately tracks the reference torque and minimizes all copper losses, resulting in significantly increased efficiency compared with conventional unitary power factor control. Moreover, the max. feasible torque is reached by taking into account rotor and stator current & voltage limits, respectively.

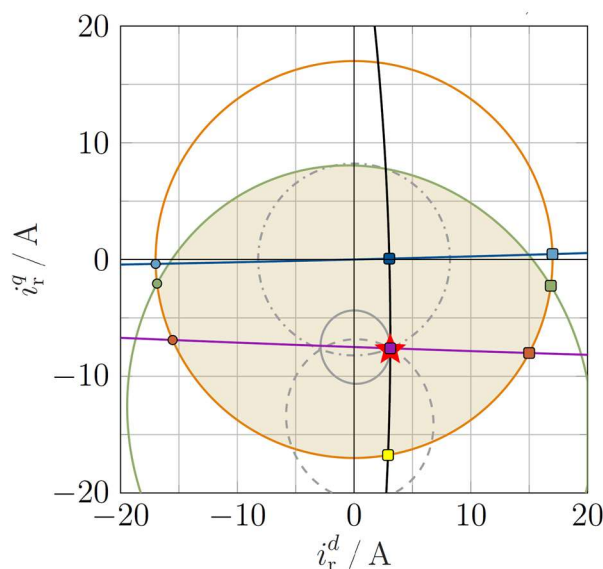


Fig. 2 Current loci of DFIG quadratics.

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Using voxel masks to assess evapotranspirative cooling from urban tree arrangements

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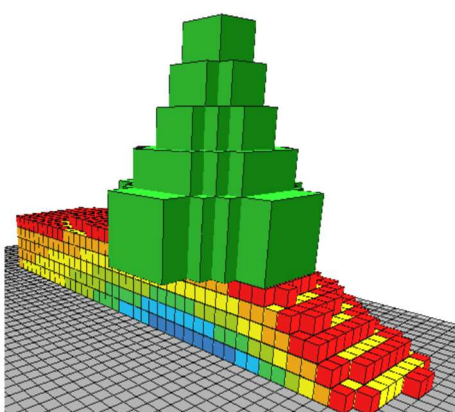


Figure 1: Cut through a resulting voxel deviation mask (potential air temperature) calculated in ENVI-met for a single tree

Evapotranspiration from urban trees is a complex process that makes calculation resource-intensive. Therefore, we propose the use of a preprocessing approach, in order to minimize calculation time. In this paper, we show the results by utilizing the voxel methodology [1]. This methodology has been used for the assessment of shading in urban environments and is extended to represent differences in air temperature caused by evapotranspiration.

The voxel masks are preprocessed using ENVI-met [2], a validated software for the calculation of outdoor parameters. The first development is carried out in an 80 x 40 x 25 meters area, where a single tree on a hot day is modeled. A second model with the same dimensions and soil but without a tree is also simulated. Afterward, both results are imported into a Pandas Dataframe using Python programming language [1]. By subtracting the values of potential air temperature, the resulting difference can be saved for every 1m³ grid cell, so-called voxel (Fig. 1).

After preprocessing the single tree voxel mask, it can be merged into a study area. As the overlay of two voxel masks cannot be added linearly, an overlapping factor has been introduced. Voxels that exceed the maximum value in the single tree mask after merging are multiplied by this factor. A good correlation has been achieved with a factor of 0.8, but more research has to be done to improve the correlation. Furthermore, temperature differences above -0.15 K are cut off, to avoid accumulation in distant areas. Validation has been carried out by simulating three overlapping trees in ENVI-met and by using the described voxel approach. Results show a maximum deviation of +/- 0.3 K, but some discontinuities at the system boundaries of the preprocessed masks (Fig. 2, x = 7). Simulation times were 4.5 hours in ENVI-met compared to 4 seconds with the voxel methodology. The proposed methodology has to be further validated by more tests and applications in urban environments. Furthermore, merging rules for overlapping and boundary voxels have to be developed. The utilization of voxel masks for assessing evapotranspiration offers a high potential for reducing simulation time while keeping results in a suitable range.

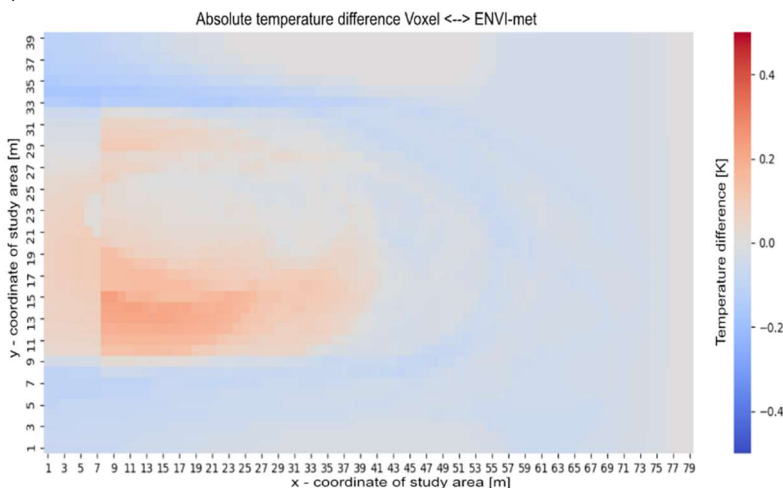


Figure 2: Validation on a test field of 3 trees simulated with ENVI-met and voxel methodology (tree positions: x = [20, 34, 48], y = [20])

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The research project 'Densification in context of climate change' is funded by Bavarian State Ministry of the Environment and Consumer Protection (StMUV) and the TUM Centre for Urban Ecology and Climate Adaption (ZSK).



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Material Design Parameters for the Generation of Hydrogen on Semiconductors from Light

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The inherent fluctuations in renewable energy sources such as wind and solar energy call for efficient energy storage and transportation methods in order to ensure a reliable energy grid. H₂ is regarded as one of the most attractive energy vectors, as it can be converted into electricity in fuel cells at high efficiencies without emitting greenhouse gases.

One way to generate H₂ is the photocatalytic conversion of alcohols. These are readily available from the fermentation of biomass, thus making this process an environmentally benign alternative to techniques employing fossil feedstocks. Similar to solar cells, solar energy is harvested in photocatalysis by semiconductors. Charge carriers are formed in the semiconductor upon illumination with sufficiently energetic light and subsequently travel to its surface, where they initiate chemical reactions. The deposition of noble metal particles on the semiconductor surface may enhance or alter the chemical reactions. Hence, these particles are referred to as co-catalysts. However, current photocatalysts still lack efficiency and “solar” H₂ is therefore economically uncompetitive. The high complexity of applied catalyst often renders a detailed elucidation of reaction mechanisms impossible, thus impeding the strategic optimization of these systems. In particular, the role of metal co-catalysts and their influence in the photocatalytic reaction are still under debate.

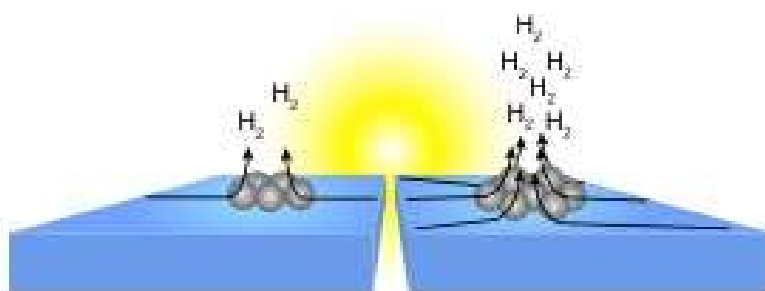


Figure 1: Photocatalytic H₂ evolution from co-catalyst clusters of different size.

In this regard, our group has only recently discovered a new mechanism for the H₂ evolution reaction on noble metal-loaded semiconductors based on detailed investigations on single crystals under highly defined reaction conditions.^[1,2] In this work, we extend those insights to material design parameters such as the co-catalyst particle size. This strategy facilitates insights into their effect on the photocatalytic performance. The respective roles of the semiconductor and the co-catalyst are elucidated in detail in the contribution “Understanding the Chemistry of Alcohol Photocatalysis for Sustainable Hydrogen Production”.

A profound understanding of the reactivity on the atomic level facilitated by such fundamental studies is important for the design and optimization of applied photocatalysts. Tailoring the co-catalyst particle size on semiconductors can help to enhance mass-specific activities in photocatalytic applications.

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Hybrid Energy Harvester based on Triboelectric Nanogenerator and Solar Cell

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Developing clean energy techniques plays a central role in the 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 continuously provide an energy source [2]. Triboelectric nanogenerator (TENG) originating from Maxwell's displacement current is a new type of energy harvesters. Due to its advantages of light-weight, low-cost, and easily fabrication, different kinds of TENG devices have been fabricated for harvesting various energies in the past years [3-4].

In the present work, a flexible hybrid energy harvester was 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 1a. Here, the gold electrode serves as both the electrode for TENG and the anode for PbS QD based solar cell. Figure 1b 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 [5]. This work may have great applications in smart home systems and internet of things.

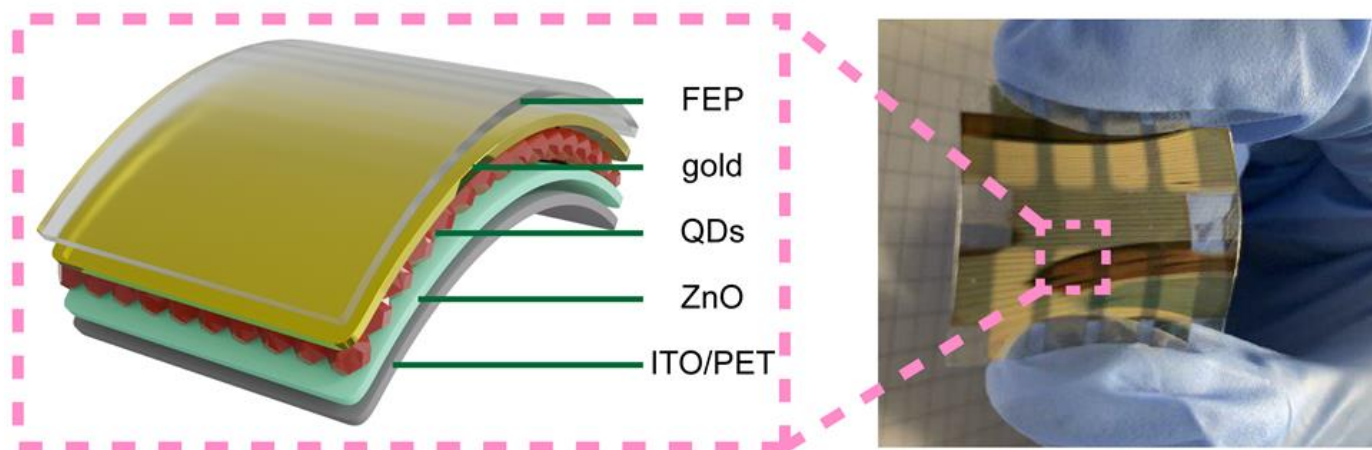


Figure 1: a) Fabricated hybrid energy harvester as sketch and b) in reality.

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Fast Lithium-Ion Conduction in the Hydride $\text{Li}_3(\text{NH}_2)_2\text{I}_{1-x}(\text{BH}_4)_x$ ($0 \leq x \leq 0.3$)

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All-solid-state batteries are considered to extend the limits of conventional lithium-ion batteries in terms of safety, cycle stability, and power density. The solid electrolyte, which is lithium-ion conducting and electronically insulating, is a key component for this technology. There are numerous different electrolyte classes based on oxides, sulfides, and phosphides, which exhibit lithium-ion conductivities up to 25 mS cm^{-1} .^[1] Recently, complex hydrides of the form $\text{M}_x(\text{M}'_y\text{H}_z)$ came into focus as a new class of solid electrolytes with high electrochemical stabilities, small densities, and relatively high ionic conductivities of 0.2 mS cm^{-1} for $\text{Li}_2(\text{NH}_2)(\text{BH}_4)$ ^[2] and 0.05 mS cm^{-1} for $\text{Li}(\text{BH}_4)_3\text{I}$ ^[3] at room temperature.

$\text{Li}_3(\text{NH}_2)_2\text{I}$ is a complex hydride in the LiNH_2 - LiI system crystallizing in the hexagonal space group $\text{P6}_3\text{mc}$ (186) with $a = 7.0911 \text{ \AA}$ and $c = 11.5096 \text{ \AA}$.^[4] Since the phase-pure synthesis of the compound was not successful till now, conductivity measurements were performed with an equimolar amount of LiNH_2 beside $\text{Li}_3(\text{NH}_2)_2\text{I}$ resulting in ionic conductivity of 0.017 mS cm^{-1} at 300 K. In addition to the phase-pure synthesis, we aim here to partially substitute I^- by BH_4^- to investigate the influence of structural changes and the presence of a further complex anion next to NH_2^- on the ionic conductivity.

In this work, we show the phase-pure synthesis of $\text{Li}_3(\text{NH}_2)_2\text{I}$ and the related substitution series $\text{Li}_3(\text{NH}_2)_2\text{I}_{1-x}(\text{BH}_4)_x$ ($0 \leq x \leq 0.3$) as well as their structural and electrochemical characterization. Crystallizing in the space group $\text{P6}_3\text{mc}$, the lattice parameters of the substitution series behave anisotropic with increasing BH_4^- content. The lithium atoms occupy tetrahedral voids, which are coordinated by three $\text{N}(\text{H}_2)^-$ anions and one $\text{I}/\text{B}(\text{H}_4)^-$ anion (Figure 1). The ionic conductivity of the series is above 0.2 mS cm^{-1} at room temperature for all four compounds, which is an order of magnitude higher than the previous value for $\text{Li}_3(\text{NH}_2)_2\text{I}$.

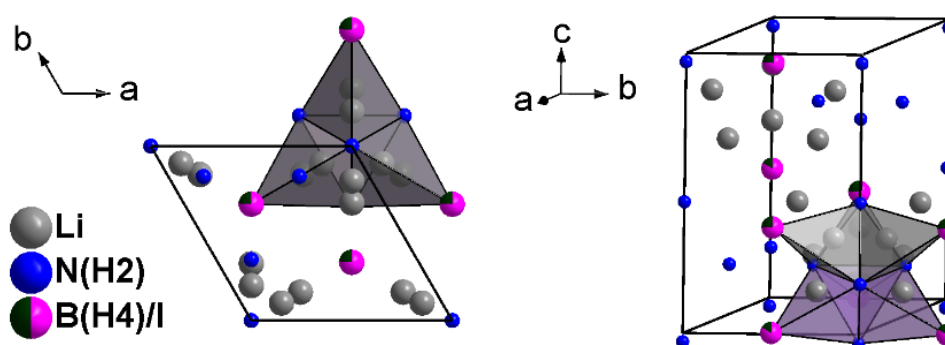


Figure 1: Crystal structure of $\text{Li}_3(\text{NH}_2)_2\text{I}_{1-x}(\text{BH}_4)_x$.

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Studies on Polymer Electrolytes for Thin Film Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) are a substantial component of the energy supply in our modern society with applications ranging from small micro batteries to larger battery packs in electric vehicles. Due to the sufficient high ionic conductivity, most commercial batteries use ionic liquids (ILs) as electrolytes for ion conduction which, however, suffer amongst other things from flammability and can cause serious damage to the end-user.

Polymer electrolytes can bypass this issue and exhibit several benefits compared to conventional liquid electrolytes and additionally can pave the way for new cell designs like thin-film geometries. Polyethylenoxid (PEO) based materials are one of the most extensively studied polymers for lithium-ion battery applications due to the superior solubility of lithium salts for example Lithium bis(trifluoromethanesulfonyl)imide (LiTFSI). However, these polymer electrolytes possess low ionic conductivities mainly due to the semi-crystalline structure which hinders the ionic motion [1]. Promising candidates as polymer electrolytes for LIBs are single ion-conducting polymer electrolytes in which the anion is covalently bonded to the polymer backbone and only the lithium cation is mobile. Hence, they theoretically achieve a transference number of unity which is accompanied with suppression of dendrite growth in battery cells with lithium metal as anode [2].

In this study, a polymer blend of PEO and the single ion conducting polymer Poly((trifluoromethane)sulfonamide lithium methacrylate) (PMTFSILi) with a ratio of $[EO]/[Li] = 10$ is fabricated and its thermal, electrical, and morphological properties are investigated.

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Lithium mobility in Highly Oriented Pyrolytic Graphite (HOPG)

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The determination of the solid-state lithium diffusion coefficient in lithium-ion batteries is an important parameter to assess whether solid-state diffusion plays a limiting role in charging/discharging the anode side of the battery electrode. Due to the complex phase transitions, the diffusion coefficient of lithium in graphite has not been precisely determined to date. Experimental investigations using different measuring methods yield results that vary over several orders of magnitude. One reason could be the inhomogeneities of conventional graphite anodes, which consist of heterogeneous graphite particles connected by polymeric binders.

The poster describes how lithium mobility in highly oriented pyrolytic graphite (HOPG) can be determined by optical studies to draw conclusions about the solid-state diffusion of Lithium in graphite. The intercalation of Lithium into graphite is a multi-stage process. Once LiC_{12} is reached, additional Li goes into the unoccupied galleries through a two-phase transition with lithium in every layer growing as the LiC_{12} phase shrinks until the fully ordered LiC_6 is obtained with the highest capacity. The LiC_6 phase is gold-colored. The propagation of the golden phase in the round HOPG sample is studied as a time- and temperature-dependent process, leading to an apparent diffusion coefficient presented in the poster.

A

$$CC = 20 \mu A$$

$$CV = 40 mV$$

B

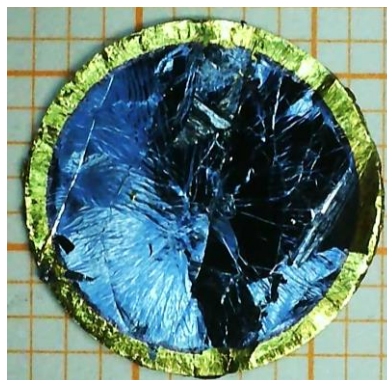


Figure 1: A) Electrochemical lithiation of the HOPG via constant current mode and subsequent constant potential charging. B) Lithiated HOPG with golden LiC_6 phase.

Testing of multi-energy management platform in a microgrid laboratory environment

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The research project "Multi-Energy Management and Aggregation Platform (MEMAP)" develops a software platform that optimizes and coordinates the energy flows in smart neighborhoods during live operation. The motivation is to enhance and use sector coupling between the heat and electricity sector and at the same time exploit synergies between the different demand profiles, generation & storage capacities of the participants in the neighborhood. This leads to a higher system efficiency and over time saves energy, costs, and CO₂ for the neighborhood as a whole. The platform connects different local Energy Management Systems (EMSs) in the neighborhood (see Figure 1). For the communication, the industrial communication protocol OPC UA is used. The platform aggregates data from these EMSs and uses the information to optimize the generation schedule. The optimized schedule is sent back to the local EMSs as setpoints for the power flows. The EMSs are responsible for implementing these setpoints autonomously in the individual devices. The model predictive controller (MPC) in the kernel of the platform is able to consider time variable prices and automatically features smart buying or selling of energy from the public grid as well as anticipatory charging and discharging of storages. Therefore, it uses internal models of the neighborhood including its devices and forecasts for the future demands, generation capacities, and prices that are provided by external sources.

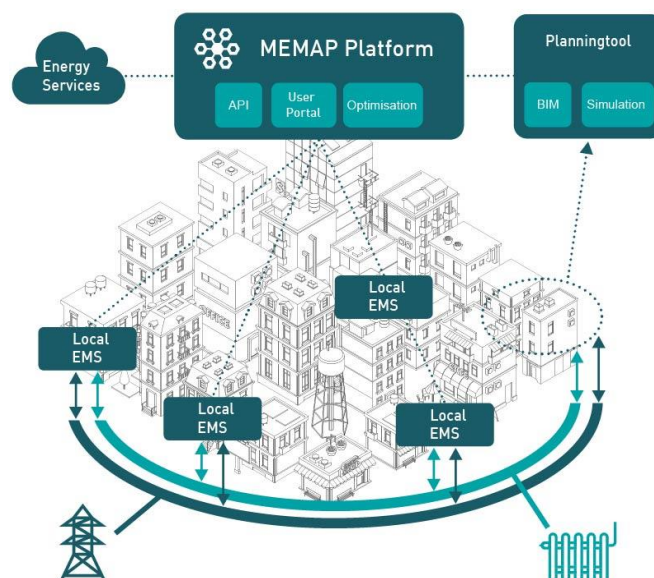


Figure 1: Concept of the MEMAP research project

As one of the first projects, the MEMAP platform is tested in the laboratory environment of the Center for Combined Smart Energy Systems (CoSES) at TUM. The Objectives of the test runs in the microgrid laboratory are a general and practical validation of the developed communication and interface concept in interaction with real devices as well as the general testing of the platform functionality and the software architecture.

A scenario with two buildings was chosen. This includes two 800 liter heat storage tanks and the two heat sinks, a condensing boiler with 21 kW output, and a CHP unit with 2 kW electrical and 5 kW thermal output. Additionally, the buildings are connected via a thermal and an electrical grid. The platform is integrated into the CoSES environment as illustrated in Figure 2. MEMAP is installed on a host computer, the simulation of the individual EMS is carried out via self-designed models. The laboratory tests run in real-time over periods of 8 to 36 hours.

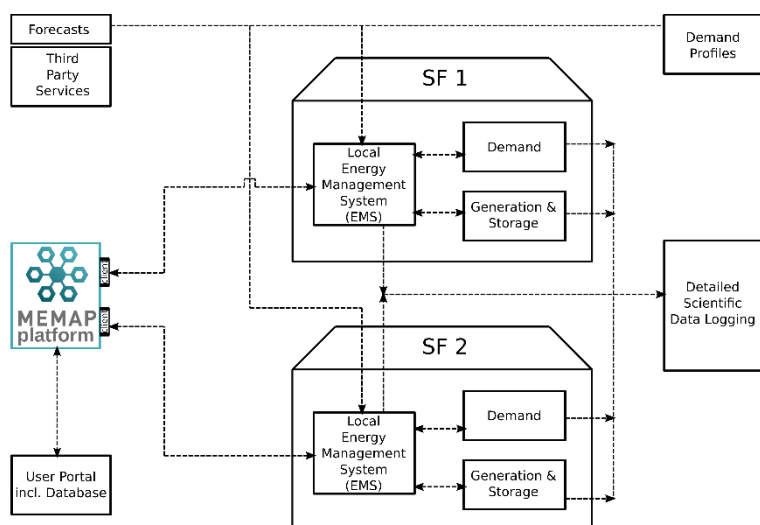


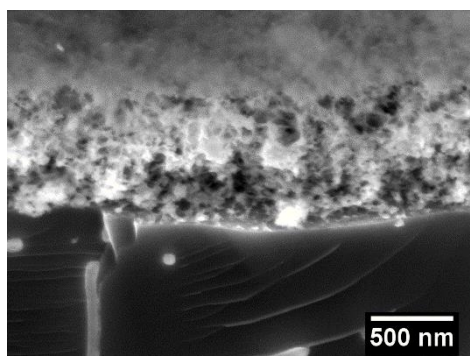
Figure 2: Integration of the MEMAP platform in the CoSES laboratory

Sol-gel derived germanium-based nanostructures

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Lithium-ion batteries (LIBs) have taken over a major role in the field of energy storage for several years. Especially in sectors such as portable devices, renewable storage systems, and especially electric vehicles this technology is already dominating the market. In order to meet the ever-increasing requirements such as durability, energy density, and manufacturing costs, it is essential to implement new performance-enhancing materials into the cell architecture. Group IV elements as Silicon (Si) and Germanium (Ge) are considered to be appealing alternatives to commercial graphite anodes due to their high energy capacity. In this respect, Si is becoming the focus of research due to the highest theoretical capacity (4200 mAh g^{-1}) and low working potential. ^[1] Additional advantages such as environmental friendliness, resource abundance, and low cost have prompted several research groups around the world to look closer into this topic. However, the cycling performance and the rate capacity of these novel anodes are still limited by the low intrinsic electron conductivity and poor Li^+ diffusivity. In addition, Ge can provide better cyclability and a dramatically improved electron conductivity into the system. But also Ge suffers from drawbacks as a comparably high price and low abundance.



One promising approach is to synthesis porous anodes instead of continuous ones. Here the surface-to-volume ratio can be increased drastically to enlarge the solid electrolyte interface by several orders of magnitude (see Figure 1). In this project, a sol-gel approach is used where the amphiphilic diblock-copolymer PS-*b*-PEO (polystyrene-block-polyethylene oxide) acts as the structuring agent. By varying the molar ratio of styrene to ethylene

Figure 1: Sketch (left) and a cross-section scanning electron microscopy image of a calcinated thin film

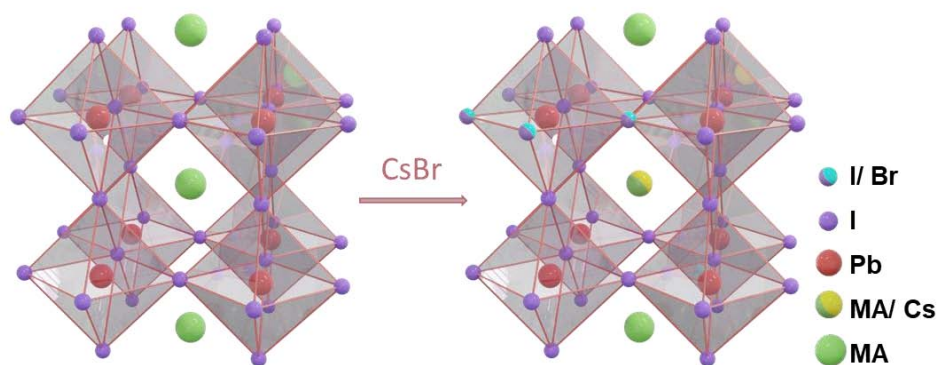
oxide one can synthesis different morphologies for any wanted purpose. Zintl clusters ($\text{K}_{12}\text{Si}_x\text{Ge}_{1-x}$) with tunable Si-Ge ratio are used as the group IV source. The thin film is additionally subjected to a butanol-toluene atmosphere for further improvement of the morphology formation. Once the solvent-treated thin film is calcinated and then washed with organic solvents to remove remaining residues, the thin film reveals its final structure as depicted in the cross-section image in Figure 1. Soon to be assembled coin cells will provide more insights into the behavior as novel anodes in LIBs.

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The Role of CsBr on Crystal Orientation and Optoelectronic Properties of MAPbI₃-based devices

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Crystal orientations are closely related to the behavior of the photogenerated charge carrier and are vital for controlling the optoelectronic properties of perovskite solar cells. Herein, we propose a facile approach to reveal the effect of lattice plane orientations on the charge carrier kinetics via constructing CsBr doped mixed-cation perovskite phases. Through grazing-

Figure 2: the evolution of active layer component after doping CsBr in the perovskite crystal

incidence wide-angle X-ray scattering (GIWAXS) measurements, we systematically investigate the crystallographic properties of mixed perovskite films in the microscopic scales and reveal the effect of the extrinsic CsBr doping on the stacking behavior of the lattice planes. Combined with transient photocurrent (TPC), transient photovoltage (TPV), and trap density of states (tDOS) characterizations, the recombination of the photo-generated charge carrier is characterized. It is demonstrated that CsBr compositional engineering can significantly affect the perovskite crystal structure in terms of the orientation of crystal planes, reduction of trap-state density, and facilitate the photo-generated charge carrier transport across the absorber and pertaining interface simultaneously. This strategy provides a unique insight into the underlying relationship among the stacking pattern of crystal planes, the photo-generated charge carrier transport, and the optoelectronic properties of solar cells.

Image-based Microstructural Analysis for the Production of Large-Format All-Solid-State Batteries

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Finding solutions for the sustainable storage of energy is one of the main challenges of the 21st century. Sulfide-based all-solid-state batteries are promising candidates among the next generation of storage technologies. Their advantages include high energy and power densities, improved long-term stability, and high safety. Due to these characteristics, sulfide-based all-solid-state batteries could be used in a wide range of products and conquer previously untapped areas of application.

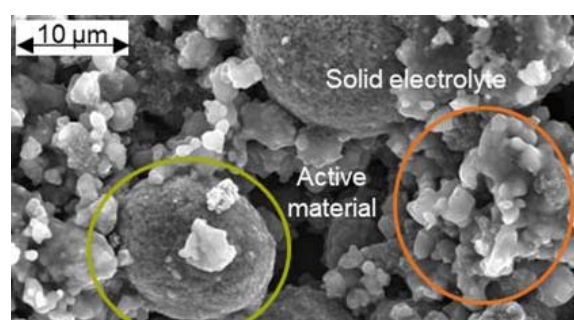


Figure 1: Microstructure of a sulfide-based composite cathode

As of today, the successful market entry of sulfide-based all-solid-state batteries was not possible, since their production technology is still in its infancy. Suitable processing routes and process parameters on large-scale production must be identified for the manufacturing of low-cost and high-quality battery cells. This poses a major challenge since most of the sulfidic materials have not yet been processed in quantities beyond laboratory scale. Besides, applicable processing routes and suitable process parameters have barely been researched yet. This relates in particular to the production of large-format sulfide-based composite cathodes.

To establish production technology for large-format composite cathodes, an analysis of the intermediate product's microstructure is conducted for various process routes and process parameters. Thereby, the key focus is on the active material and the sulfide-based solid electrolyte particles (Figure 1). The distribution of the former is of importance since it influences the electrochemical load on the composite cathode during operation. The solid electrolyte particles are of particular interest since they enable ionic conductivity within the composite cathode. They must be distributed homogeneously for a uniform ionic flux density, and have sufficient contact with all other particles.

In the first step, the microstructure resulting from the different processing routes and process steps is visualized using a scanning electron microscope. Afterward, based on the evaluation of the homogeneity of the particle distributions and contacts, assessments of processing routes and parameters are made. This is assisted by semi-automated intelligent multi-step image evaluation algorithms enabling the analysis of large quantities of microstructural images (Figure 2).

Suitable processing routes were obtained by this approach.

This includes the finding, that the homogeneity of the active material distribution in the composite cathode is hardly influenced by the chosen process steps. However, their contact with the solid electrolyte particles strongly depends on both the process steps and the process parameters. The same was observed regarding the distribution and contact of the solid electrolyte particles.

As a result, suitable pilot-scale processing routes and their parameters were identified. The findings strengthen and deepen the understanding of the production of sulfide-based composite cathodes for all-solid-state batteries.

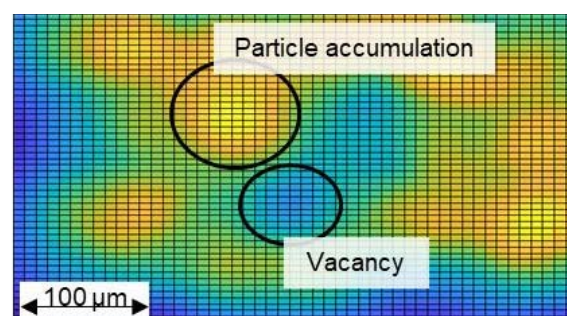


Figure 2: Evaluation of the homogeneity of the distribution of active material particles

Sol-gel based tailored lithium-ion battery electrodes

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Silicon-based materials have been considered one of the most promising candidates for the next-generation lithium-ion battery anodes. The current commercially used anode material, graphite, exhibits great mechanical properties; however, it has reached its limits regarding energy density and its specific capacity (372 mAh/g). The novel materials are being developed to meet the increasing demand on the efficiency and reliability of the Li-ion batteries for electronic devices, electric vehicles, and energy storage applications. Therefore, silicon is a great alternative, thanks to its low cost, non-toxicity, and high theoretical gravimetric capacity (4200 mAh/g).

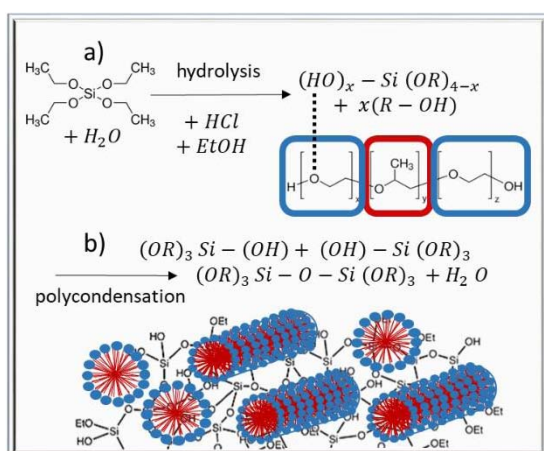


Figure 1: Mechanism of the sol-gel method: a) hydrolysis of the silica precursor & hydrogen-bond interaction between the hydrolyzed precursor and PEG block; b) self assembly of the polymer & polycondensation of the silica precursor

triblock copolymer is used as a template. The mechanism of the method is schematically shown in Figure 1. In general, the use of block copolymers as the structuring agents is one of the most promising choices, thanks to their high degree of order, low cost, and low toxicity. The starting solution is coated onto the cleaned Si substrates and the template removal is done by calcination at high temperature (400 °C). The properties of the thin films can be tuned by adjusting the synthesis conditions such as concentration of reaction compounds (e.g. silica precursor, polymer, catalyst), choice of the deposition technique (e.g. spin coating, printing), or choice of the final calcination step (air vs. inert atmosphere). The aim is to reach the desired thickness, porosity, conductivity, and mechanical stability for the successful Li-ion battery anode application. Thin films are characterized by scanning electron microscopy (SEM), grazing-incidence small-angle X-ray scattering (GISAXS), X-ray diffraction, impedance spectroscopy, and profilometry measurements. An example of the mesoporous microstructure of a Si-based thin film is shown in Figure 2.

However, silicon suffers from the large volume expansion and therefore stress generation upon lithiation and delithiation process during battery cycling. This can lead to the degradation of anode material, loss of active Li, overall battery capacity loss, and poor cycling stability. There have been great efforts made to address these problems by designing and synthesizing structurally stable Si-based anode materials that can accommodate the volume changes and buffer the developed mechanical stress. One of the many concepts is to design porous Si-based materials, which can exhibit these desired properties.

The aim of this work is the optimization of copolymer-assisted sol-gel synthesis of mesoporous silica thin films. This wet chemical method consists of the formation of the organic-inorganic composites by a self-assembly mechanism, where the organic phase (polymer) serves as a template for the inorganic structure (silica). The tetraethoxysilane (TEOS) is used as a silica precursor and the poly(ethylene glycol)-block-poly(propylene glycol)-block-poly(ethylene glycol) (PEG-b-PPG-b-PEG) non-ionic

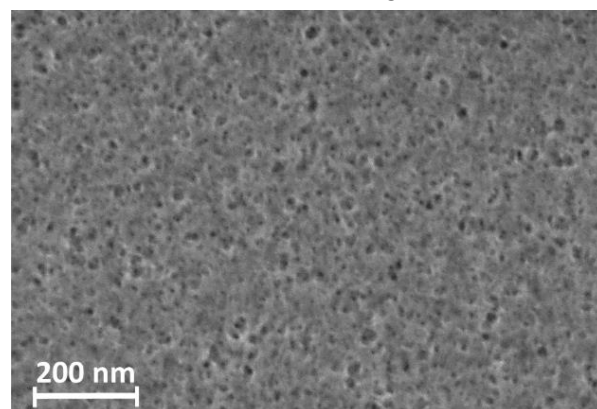


Figure 2: SEM image of the mesoporous Si thin films

Printed Organic Solar Cells

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Organic solar cells (OSCs) are one of the most promising candidates for next-generation photovoltaics due to their increasing improvement in the power conversion efficiency (PCE) and the great advantages they can offer such as low-cost fabrication, mechanical flexibility, low weight, and transparency.

OSCs are frequently based on blends of electron-donor and fullerene electron-acceptor materials that form bulk heterojunctions (BHJs) in such devices. However, recent research has focused on organic non-fullerene acceptors due to several enhanced properties, such as greater thermal stability and photochemical stability, as well as longer device lifetimes [1]. Moreover, OSCs based on non-fullerene acceptors have shown a considerable increase in device performance, reaching PCEs more than 18% [2].

In comparison with the classical rigid silicon solar cells, the solution-based manufacturing processes of OSCs such as spray coating and printing allow more viable means of production. Spray coating and printing, at the same time, enable OSCs to be used in new and more versatile applications, where different architecture and devices need to be covered with thin, light, flexible solar cells, for instance, smart windows, foldable smart roofs, aircraft, and several space technologies.

In recent years, the use of printing methods is increasing as it represents a great potential for large-scale fabrication processes. However, printing involves complex evolutions of the organic thin-film structure and morphology. Thus, morphology characterization is needed to study the printed nanostructured films. For this, we perform grazing-incidence X-ray scattering (GIXS) for the analysis of crystal structure and their domains of the printed polymer films. For this work, we use BTP-4F as a non-fullerene acceptor and we study the BHJs of the built OSCs with different organic solvents to analyze their effect on the morphology of the films.

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endemo – Energy Demand Modeling for Europe

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Energy efficiency measures on the demand side play an important role in achieving the ambitious climate and resource targets. However, the subject of research in the past was energy generation, which resulted in a large number of model activities for the creation of energy scenarios on the supply side. In contrast, there are few advanced approaches and models for mapping the demand side. In order to be able to estimate future energy scenarios, it is necessary to investigate future demand-side developments and integrate them as an essential component in energy system models.^[1]

The developed tool *endemo* (**E**nergy **D**emand **M**odeling) enables statements to be made about demand-side developments for electricity, heat, and hydrogen in the sectors of industry, households, transport as well as commercial, trade, and services (CTS). Figure 1 shows an exemplary overview of the model. Currently, spatial resolution is on the country level covering the investigation area of Europe 28 (without Malta, Cyprus, Lithuania, Estonia; including Switzerland, Iceland, Norway, Serbia, Montenegro, North Macedonia, Bosnia, and Herzegovina).

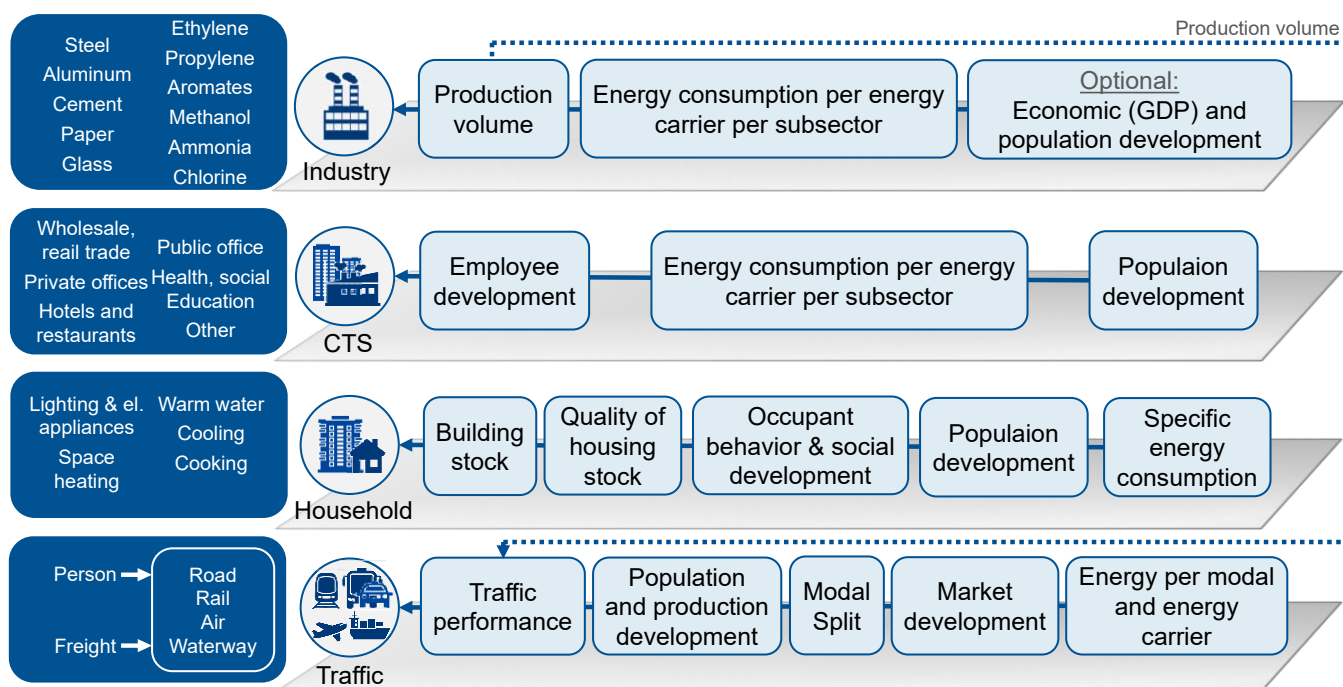


Figure 1: Exemplary overview of the developed overall method of energy demand modeling

By means of the time series profiles stored in the model, in addition to the annual demand, an hourly resolution of the output at subsector level is also possible. The calculations considering impact factors such as process and feedstock substitutions, efficiency developments, and best available technology, as well as political and market changes. The forecasts calculations for each sector include technical, economic, and social development parameters.

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Conductive Polymer Coating of NMC Cathode Material

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Nowadays, lithium-ion batteries play a major role in our lives and the importance of energy storage increases with each year. Equally important as high energy densities and good performance is the safety aspect of lithium-ion batteries. Most of the commercially available batteries are using liquid electrolytes that show high ionic conductivities resulting in a good performance. However, liquid electrolytes are flammable, can leak, become unstable at higher temperatures, and suffer under Li dendrite growth ultimately causing short circuits and thermal runaway in case of abuse.

By using inorganic solid electrolytes or polymer electrolytes, the safety of the lithium-ion battery cell can be increased at the cost of reduced performance. The major problem is the contact between electrolyte and cathode material. Unlike liquid electrolytes, the solid electrolyte cannot fill the voids within the porous electrode, which results in high interfacial resistances.

One mitigation strategy is to coat the surfaces of the electrode particles. Conductive polymer coatings on the cathode material can both improve the structural stability of transition metal oxide cathodes and improve the interfacial contact between electrode and electrolyte. Previous studies showed enhanced electrochemical performances for coated $\text{LiNi}_{1-x-y}\text{Mn}_x\text{Co}_y\text{O}_2$ (NMC) cathode materials in lithium-ion batteries. [1] For example, a conductive coating with polypyrrole (PPy) and Li_3PO_4 improved the cyclic behavior and rate capabilities and combining the two approaches yielded even better results. [2]

Here, NMC particles are coated with a conductive polymer using solution casting and will be compared to a conventional NMC cathode. The coating is examined with microscopy techniques and the ionic conductivity is measured using electrochemical impedance spectroscopy. The rate capability and the cycling performance are studied in coin cells consisting of the coated NMC, a polymer electrolyte, and a Li metal anode.

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Silylated Ge-Clusters as Precursors for Porous Ge/C-Thin Films with Tunable Crystallinity

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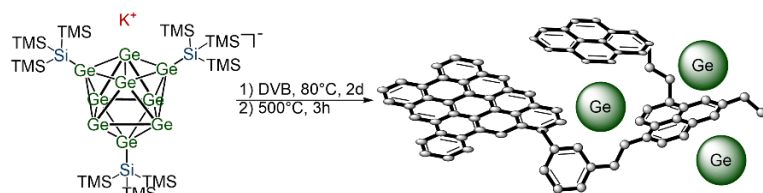


Figure 1: Synthesis procedure from TSG to C/Ge-nanocomposites.

Germanium (Ge)-based materials have gained a lot of attention as potential anodes for lithium-ion batteries because of their high theoretical gravimetric capacity (1624 mAh g^{-1}).^[1] Thus, much research has been devoted to cost-effective solution-based synthesis routes of nano-architected Ge in the past few decades. Recently, we have shown that macroporous Ge inverse opal films have potential applications as anode materials in lithium-ion batteries.^[2] However, the cycling stability of those materials remains challenging mainly due to pulverization of the active material. The structural integrity of Ge can be prolonged by using carbon matrixes. Additionally, carbon matrixes can also prevent the surface oxidation of nanostructured amorphous Ge with high surface areas.^[3] Overall carbon matrixes have the capability to greatly retard any surface degradation during storage and strongly improve cycling stability, making this a practical and promising strategy for further investigations.

Herein we report on the fabrication and characterization of porous germanium- and carbon-based nanostructured thin-film composites. The synthesis is achieved from solution mixtures with divinylbenzene (DVB) as the carbon precursor, tris-silylated nonagermanide clusters (TSG) as the germanium precursor, and a common organic solvent such as acetonitrile, tetrahydrofuran, acetone, toluene, and dimethylsulfoxide (DMSO) to further introduce pores into the Ge/C-composite (Figure 1). Scanning electron microscope (SEM) images revealed the important role of solvents in the preparation of homogenous thin films. High-temperature boiling solvents such as toluene or DMSO lead to the formation of cracks inside the material. In contrast, low-temperature boiling solvents lead to the formation of homogenous thin films with porous in the 500 nm range (Figure 2). The elemental composition and crystallinity of the material are investigated by energy-dispersive X-ray spectroscopy and powder X-ray diffraction/Raman spectroscopy, respectively. The crystallinity of Ge is tunable from amorphous to crystalline α -Ge with increasing temperature from 500 to 1000°C. Furthermore, TGA analysis under inert conditions indicates that the decomposition of DVB to amorphous carbon is stabilized by the presence of TSG.

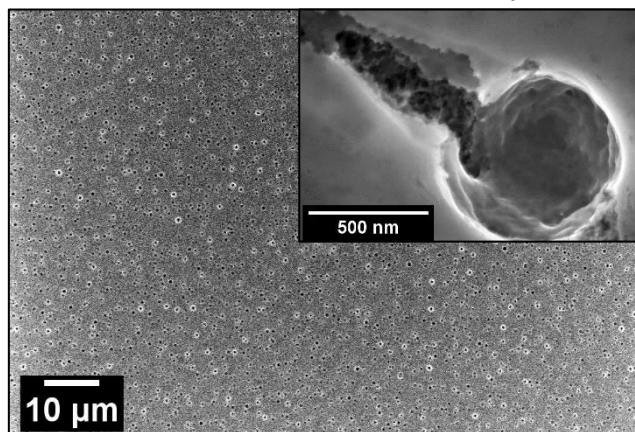


Figure 2: SEM microimages of porous C/Ge-thin films on Si-wafers.

Lastly, a combined ex-situ-¹H NMR/GC-MS and PXRD study of annealed TSG reveals parts of the decomposition path of the tris-silylated Ge₉-clusters to elemental Ge and volatile tetrakis-trimethylsilyl-silane as well as hexakis-trimethyl-disilane.

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New Frequency Adaptive Observer for Fast Estimation of Fundamental Phase Parameters

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Motivation

In power systems like overhead power lines, the voltage amplitude, phase, and frequency must match certain restrictions to ensure a stable operating grid. To keep these parameters in the allowed range, it is necessary to estimate them online. These estimates then can be used for compensation strategies where a faster estimation allows for a faster reaction.

Methodology

Usually, the well-known *Second Order Generalized Integrator (SOGI)* [1] combined with a *Frequency Locked Loop (FLL)* [2] is used to deal with this task. This structure is called a *standard Frequency Adaptive Observer (sFAO)*. Unfortunately, the sFAO has the disadvantage of speed limitation, i.e. the algorithm requires at least a certain time frame to estimate amplitude, phase, and frequency correctly. To set the required time frame to a desired value, this poster proposes a new method for detecting amplitude, phase, and frequency, called the *transformation-based Frequency Adaptive Observer (tFAO)*. The main difference between the sFAO and the tFAO is that the sFAO can be separated into SOGI and FLL where the tFAO cannot. The tFAO is able to estimate the parameters within a predefined time frame where the settling time can be specified by pole placement. In Figure 1, the proposed tFAO is shown.

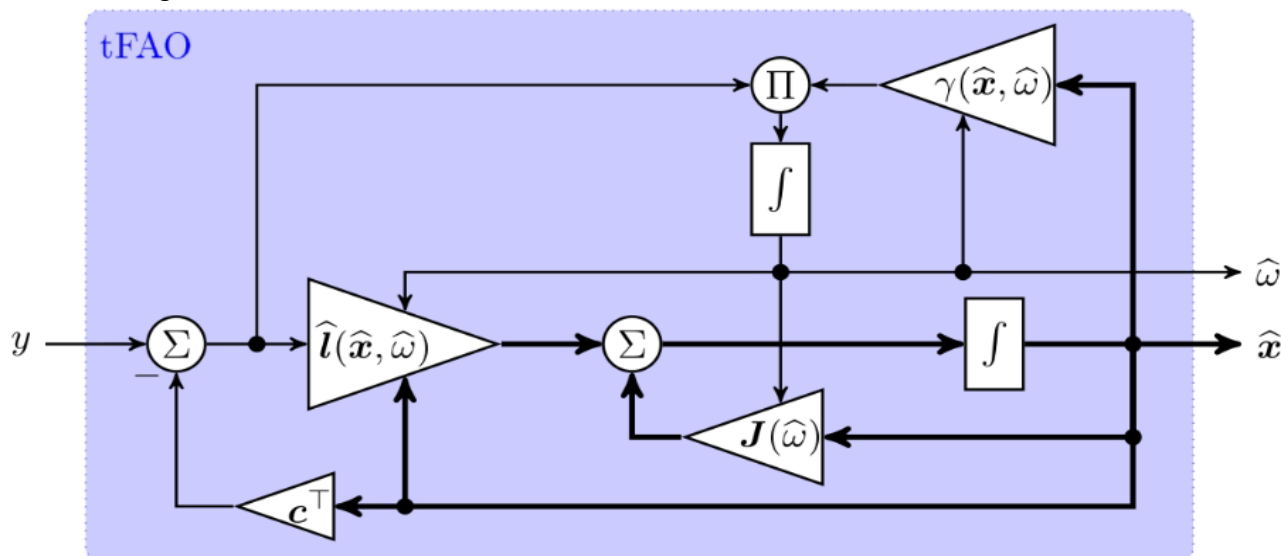


Figure 1: The proposed tFAO.

Results

Simulation results show that the tFAO, in comparison to the sFAO, is able to estimate amplitude, phase, and frequency much faster.

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E-mobility platform for the CoSES laboratory

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The CoSES research group is equipped with a microgrid laboratory designed to explore and develop solutions for sector coupling: electricity, heat, and mobility. For the latter, the lab has at its disposal the EV-charging stations mounted in front of the ZEI building. These are typical charging columns employed for public use; integrated with an *Accounting Control Unit* (ACU) they can communicate with a central management system for customer authentication, sharing metering values to ultimately cash the consumers, running remote diagnostics, and if desired handling intelligent load management. However, this interface has not yet been implemented with these chargers, leaving any of these features out of use for the lab.

The goal of this project is to establish a communication link between the EV-chargers and the lab and to incorporate these into the CoSES ecosystem. First, a backend central management system is set up to exchange messages back and forth with the chargers. As a common language serves the *Open Charge Point Protocol* (OCPP), a widely adopted standard for operating charging infrastructure. The charging station management system is then configured to forward data to the CoSES IoT platform, providing real-time visualizations of the power consumption of charging vehicles. By logging the metering values, a dataset of EV charging profiles is generated, which can then be shared as open access data with other researchers for further use. Lastly, the backend is provided with an API to bind in-house developed smart *Energy Management Systems* (EMS) and offer them control over the EV load management.

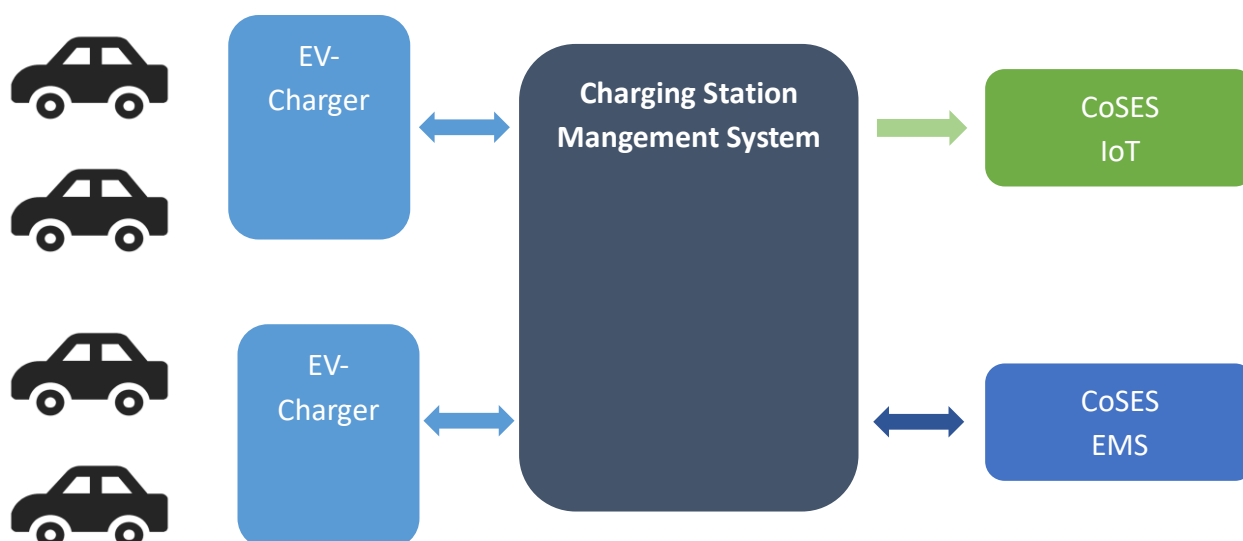


Figure 1: CoSES EV-platform and communication architecture

Exfoliated carbon nitride/hydrogen-bonded organic pigment heterostructures for hydrogen peroxide generation

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Renewable green energy is now firmly embedded in people's daily lives. Nobody is surprised using hydrogen instead of petrol anymore. The challenge becomes not in the process of generation of green fuel, but in the technique of its further storage for certain needs. Hydrogen peroxide is a high-energy compound, immiscible in water, convenient to store, and transport in the form of aqueous solutions. The industrial method of H₂O₂ synthesis is based on the anthraquinone process, requiring enormous energy consumption and is not environmentally friendly. Therefore, photocatalytic synthesis of H₂O₂ involving non-toxic materials seems to offer a good option for an alternative synthetic method.

We present in our work a new method of hydrogen peroxide generation based on heterostructures of exfoliated carbon nitride with industrial hydrogen-bonded pigments (epindolidione - Epi, quinacridone - QNC, phthalocyanine – H₂Pc, indanthrone - Ind). The application of pigments in chemical syntheses is always a challenge associated with extremely low solubility due to the presence of strong intermolecular hydrogen bonds. Strong acids or bases provide a way to break the intermolecular hydrogen bonds, making the pigments highly soluble. Conversely, strong acids and bases are used to exfoliate graphitic carbon nitride. Therefore, using TMAH (tetramethylammonium hydroxide) as a strong base, heterostructures of carbon nitride with pigments were obtained. The amount of H₂O₂ photogenerated by the heterostructures is different for various pH (2, 7, and 12) and is associated with protonation or deprotonation of the heterostructures and as a result of electrostatic repulsion between the carbon nitride and pigments. Optimization of photocatalysis conditions involving the sacrificial electron donor (TEOA - triethanolamine) shows superior activity for the ex-C₃N₄/Epi (1436 μM·h⁻¹) system compared to other heterostructures: ex-C₃N₄/QNC – 775 μM·h⁻¹, ex-C₃N₄/H₂Pc – 456 μM·h⁻¹ and ex-C₃N₄/Ind – 443 μM·h⁻¹. In the reaction with bare exfoliated carbon nitride, the amount of photogenerated H₂O₂ is 170 μM·h⁻¹. Series of tests demonstrating the stability of the heterostructures in the photocatalytic system was performed and found that the activity decreases after 5 cycles by only 94% compared to the initial hydrogen peroxide concentration. Solar energy to H₂O₂ conversion efficiency for ex-C₃N₄/Epi is 0.136 %. In fact, the formed heterostructures based on carbon nitride with daily-life pigments display improved photocatalytic properties compared to bare ex-C₃N₄. Furthermore, this research reveals a simple and feasible synthesis of a photocatalyst to produce H₂O₂ electrochemical cells.

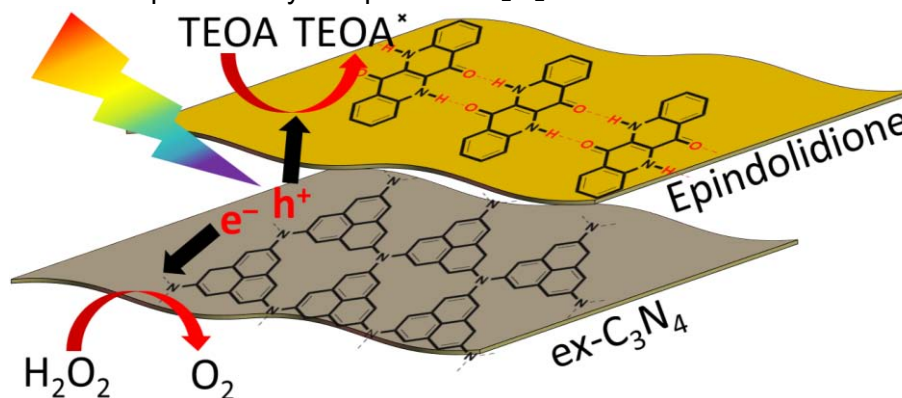


Figure 1: Schematic demonstration of photocatalytic process for H₂O₂ by using ex-C₃N₄/Epi.

Effects of oxygen plasma on the nanoscale morphology of polyelectrolyte-gold interfaces during gold sputtering

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Sulfobetaine-based polyelectrolytes have found use as efficient interlayers in organic photovoltaics. However, their polymer-metal interfacial morphology remains elusive. Moreover, plasma pretreatment of organic solar cells can bypass operational degradation due to prolonged light exposure and increase solar cell performance. We utilize in-situ grazing incidence small angle X-ray scattering, to probe the evolution of gold cluster growth on thin polysulfobetaine films during metal sputtering, the latter being an industrially-relevant fabrication technique with high precision in the control of metal layer development. We report distinct differences on the nanostructural morphology of sputtered gold with and without oxygen plasma pretreatment. Our results are corroborated by x-ray reflectivity where we identify differences in polymer-metal intermixing across the film's cross-section. Our results in these simplified polymer-metal thin films bear strong potential for optimization in the design of polymer-metal interfaces for high performance.

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Future power grid planning in urban distribution system structures

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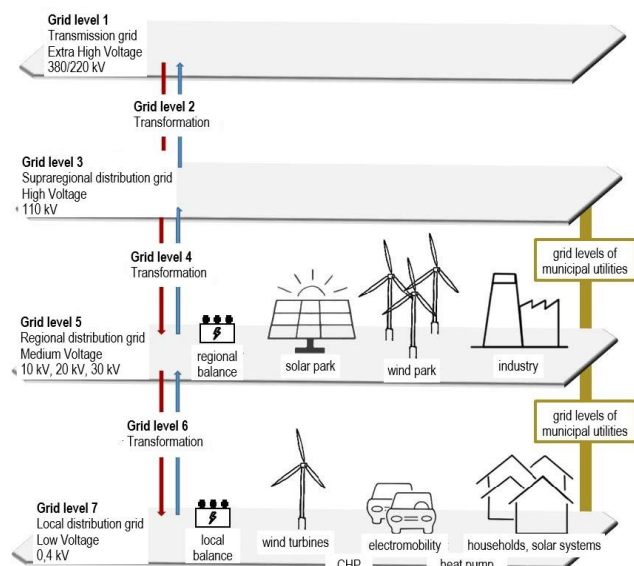


Figure 1: Grid levels in German power grid

The change in electrical energy supply in Germany away from conventional power plants towards renewable energies is driving electrical system operators to explore and validate new possibilities for planning and operating the German power grid. With the steady increase in decentralized energy systems and the increasing, politically driven electrification of the transport and heating sector, the changes in the regional and local distribution systems with grid levels 4-7 (Fig. 1) are greatest. This applies to the grid areas of many municipal utilities.

As part of the Bavarian research association "Energy - Sector Coupling and Micro-grids" (short: STROM), the OTH Regensburg, together with the municipal utilities Forchheim and Waldmünchen, have set themselves the goal of developing a technically and economically sustainable grid planning for urban distribution system structures. In doing so, scenarios for the future development of the loads and generation units, the

e-mobility and the CHP systems in the grid areas of the municipal utilities are considered. The coupling of the electricity, transport and heating sectors plays a central role in the research network and studies should show what effects this coupling has on the power grid and what changes result in the grid topology as well as in the behavior of the connected customers. Finally, recommendations for action are to be derived from the project results and guidelines for distribution system operators are to be developed.

After digitalization and validation of the urban distribution systems, load flow simulations should show whether current or voltage-related problems arise when considering the grid development scenarios and how problems can be solved technically and economically effectively with previously defined grid expansion and grid optimization measures. For a wide range of solutions and for comparison reasons, conventional and innovative solution options will be considered. One focus of the research work is the investigation of the potential for reducing peak loads with the use of an electrical storage system as a grid equipment. With consideration of the grid fee system, effects on the composition of grid fees (e.g. changes in the actual avoiding power) should be investigated and optimization potentials identified.

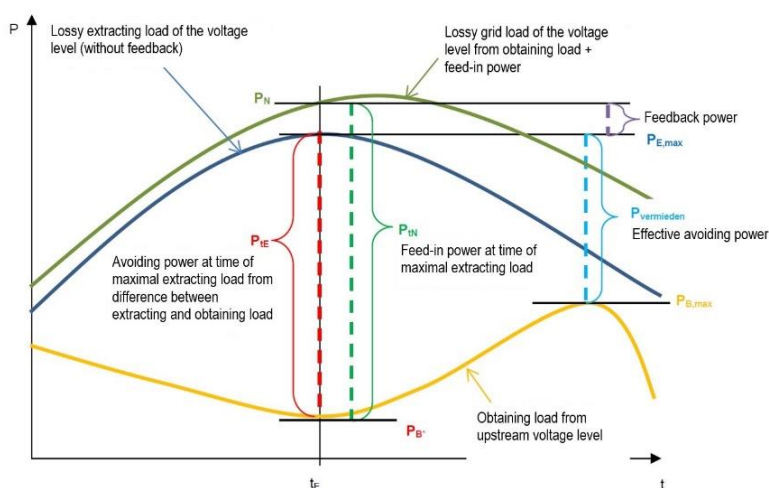


Figure 2: Illustration of avoiding power (Reference: https://www.regulierungskammer-bayern.de/veroeffentlichungen/2021-03-16_Tool_vermiedene_Netzentgelte_fuer_StromNB.xlsm)

100 % Renewable Energies for Bavaria

Potentials and structures of a full supply in the sectors electricity, heat and mobility

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The study "100 % Renewable Energies for Bavaria" deals with the scenario of a completely renewable energy supply for Bavaria in 2040. The basic scenario developed is based on the assumption of a halving of energy demand in the electricity, heating and transport sectors. The remaining demands are covered exclusively by renewable energy sources. A mathematical optimization model was used to analyze for various sub-scenarios which technologies should be used for this purpose and to what extent. In this way, important insights were gained into the functioning and optimal structure of completely renewable energy systems.

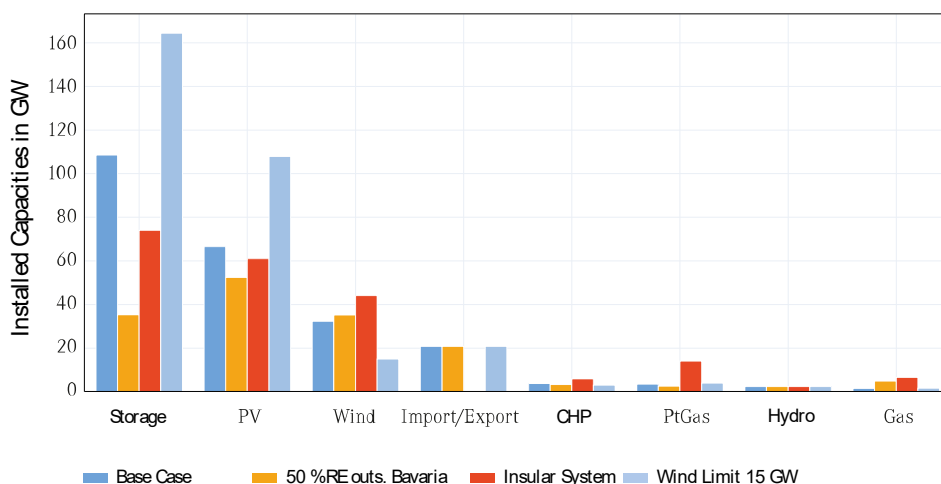


Figure 1: Installed electrical power of technologies for different scenarios

The regional characteristics of Bavaria play an important role in optimizing the energy system. The average solar irradiation in Bavaria is higher than in the rest of Germany. Photovoltaic systems achieve correspondingly high energy yields. The potential for wind power, on the other hand, is limited by geographic conditions. In addition to analyzing the actual area potential, a sub-scenario with limited use of wind power was therefore also created to investigate the possible effects of this limitation. Regional conditions have an even more decisive effect on the heating sector. Here, supply must always take place close to the consumer. Therefore Bavaria was split up into different type areas in the energy model. These type areas differ, for example, in their population density or the local potential for deep hydrothermal geothermal energy. Only in the transport sector the assumption was made that Bavaria does not differ from the rest of Germany.

Lifetime Consumption Assessment for Conventional Power Plants

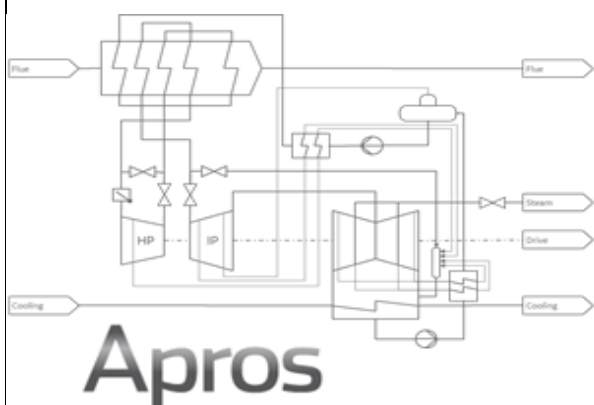
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A rapidly growing integration of renewables and the intrinsic uncertainties in their generation imposes significant limitations on operation of conventional thermal power plants. The imposed restrictions lead to a decreased utilization of such units in presence of renewable generation and subsequently changing their role in supply from the base-load to load-balancing operation. The requirements for the load-balancing operation are challenging for such conventional units, as they are designed for the base-load operation. On the other hand, the load-balancing operation requires the unit to undergo fast, repetitive and significant load changes and even frequent shutdowns and start-ups. Such dynamic operation can in turn lead to a higher lifetime consumption of the unit or even a degraded operation.

This study is part of Turbo-Reflex grant agreement No. 764545, an EU project that aims to study the aforementioned issues by providing technology upgrades to retrofit the existing power plants, enabling flexible operation without imposing impacts on lifetime consumption, costs and emissions.

Figure 1: Reference power plant

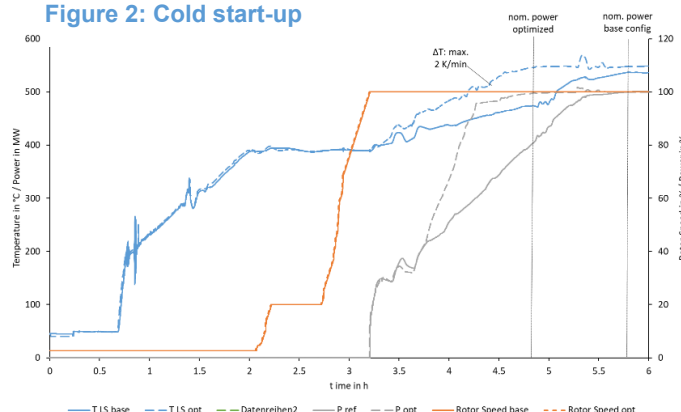


A dynamic model of a reference 870MW coal fired power plant (Figure 1) was simulated in Apros, which is a simulation environment that allows for simulating both the process and the control side, so that realistic operational scenarios can be evaluated. Additionally, a lifetime analysis module was developed internally to calculate the stress of the critical parts of the boiler according to the EN12952, as well as the turbine stress during start-ups and load operations. The developed module, operating in real time within the simulation model, allows for calculating and monitoring the current lifetime consumption and potentially reacting on it.

Special attention was given to a faster cold start-up, i.e. the starting of the plant after more than 48 hours of standstill. The improvements realized by partners in Turbo-Reflex allowed for an assessment on a potential improvement to the maximum allowable temperature gradients of the turbine. The developed model coupled with the new module was then used to judge the effect of such an increase on different critical components.

The results presented in Figure 2 show the reduction of the cold start-up time because of the increase in the turbine start-up gradient, which serves an increased flexibility. Additionally, it can be noticed that a faster start-up does not raise the maximum stress on the boiler; however, it does on the turbine. Hence, it demonstrates that the boiler is not the bottleneck when a faster start-up is desired. Instead, the limiting factor is the turbine and a higher lifetime consumption is to be expected in this component.

Figure 2: Cold start-up



What Factors Influencing the Adoption of Green Hydrogen: A Global Perspective

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By 2021 almost 200 countries, accounting for ~97% of the global carbon emissions, have set carbon reduction targets. Addressing the climate change problems, countries introduce and expand their policies supporting the development of renewable energy sources (RE), which should substitute fossil fuels and reduce the global carbon footprint. Studies focusing on the RE generation potential and challenges associated with the adoption of RE technologies suggest that hydrogen would play a pivotal role in the future energy system. The literature on the competing hydrogen technologies and potential use of that low-carbon resource is fast-growing, but analyses of incentives for hydrogen technologies adoption and competition are still scarce. We are filling in the gap by focusing on the two interrelated questions: 1) which regions have incentives to adopt hydrogen to support RE and which might need hydrogen to import the green energy and 2) what may help boost the competitiveness of the green hydrogen besides technological efficiency.

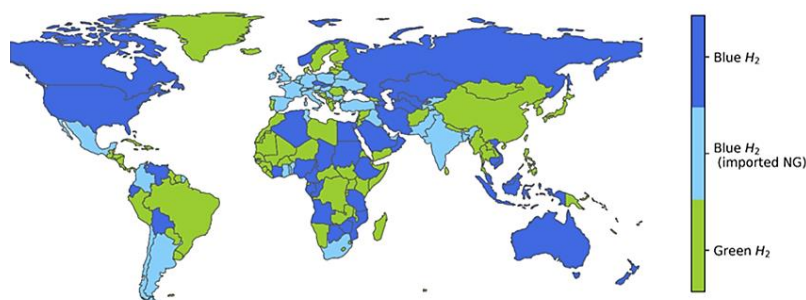


Figure 1: Countries colored by the least marginal cost H2 technology

We start our study by analyzing the RE generation potential around the world and the primary energy consumption. The compiled database enables us to reveal which regions might not be able to substitute their current fossil energy consumption with the domestically available RE resource. Hence, we establish which countries are likely to import green energy, using hydrogen or hydrogen-derived green ammonia for that.

Next, we develop a hydrogen market model with the differentiated demand for green vs. fossil-energy-based hydrogen. We solve the model to identify the key factors affecting the technology competition, incl. efficiency, input prices, demand elasticity. We highlight that the marginal costs for RE may depend on the wholesale power price and hence, natural gas. On the other hand, the cost for non-green H2 depend on carbon prices.

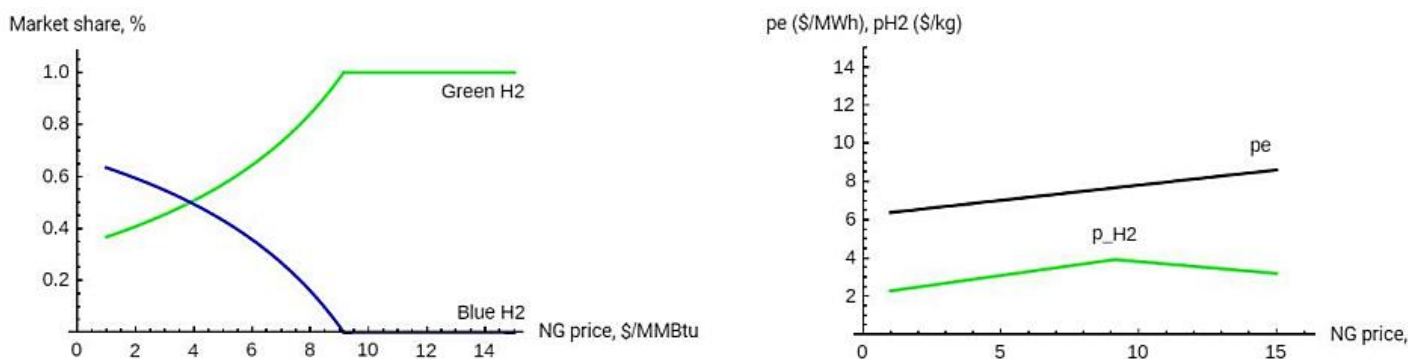


Figure 2: Results for the future hydrogen market simulations for the German market with more RE and carbon price.

We explore the role of other parameters affecting the costs, such as transportation costs, which we include into the model to run simulations. The results help us understand which market and policy instruments are most useful to promote green hydrogen technology and, how the requirements for the technology efficiency may change over time. Thus, we find that increasing renewable generation and reducing its costs is much more efficient in promoting green hydrogen than raising carbon price or tax payments. The adoption of RE could also be accompanied by an increase in the market size while decreasing H2 price. In contrast, higher carbon payments would not support the hydrogen market growth and make hydrogen more expensive. Finally, we highlight the importance of transportation costs and location of H2 facilities, suggesting that hydrogen plants located closer to the market would have a competitive advantage.