

Shaping a Sustainable Energy Future

9th Colloquium of the Munich School of Engineering
August 1, 2019



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The Swedish scientist Hans Rosling gives in his book "Factfulness" a number of very strong arguments that the world is continuously becoming better. Certainly, the globally increasing life expectancy is the strongest argument followed by many other indicators like the reduction of the very poor, the better access to education for women and the rapid decrease of children per woman. His central argument is that more and more people participate in the global economy and that the division between poor and rich, the developing and developed world is no longer valid. The past decades have seen a rapid catch-up of many world regions, especially in Asia. He argues that in preindustrial societies the price for a low population increase was the death of many children while we soon might reach a new equilibrium which is mainly driven by low birth rates which are the result of economic success and better education especially of women. Still this new equilibrium will be reached at 10-11 billion humans globally. Most of the progresses Mr. Rosling quotes are based on the intensive use of fossil fuels, the transition to renewable technologies is certainly possible but requires major efforts in the coming years. The efforts in Germany and Europe should hence be ramped up. A convincing solution for a sustainable energy system is a major step which is missing yet and once it is done it is rather likely that indicators like life expectancy will increase even more. The MSE colloquium is a very good occasion for an annual bookkeeping. Let's hope that the balance for the energy research in Bavaria is also positive so that we can also spread a well justified optimism.

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 **Geothermal-Alliance Bavaria** combines interdisciplinary research strategies in order to strengthen deep geothermal as a sustainable and controllable source of renewable energy.

- In the **Center for Power Generation** the efficiency and the environmental sustainability of existing and future power plants is increased and improved by modern and innovative technologies.
- 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.
- The **Science Center for Electromobility** contains a wide spectrum of topics from fundamental battery research, development and design of electric vehicles as well as future mobility concepts.
- 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 **Combined Smart Energy Systems Center** focuses on modeling the interdependency of electricity distribution, heat and communication networks. The goal of the center is to develop strategies for integrating extensive distributed energy sources in the energy grid of the future, the smart micro grid.

9th Energy Colloquium of the Munich School of Engineering

Shaping a Sustainable Energy Future

August 01, 2019 – 8:30 a.m. to 8:00 p.m.
TUM – Quantum, Garching-Hochbrück

8:30 – 9:00 a.m.

Registration

9:00 – 9:15 a.m.

Opening: Prof. Thomas Hamacher

Director, Munich School of Engineering, TUM

9:15 – 9:45 a.m.

Keynote: Challenges and Approaches for a Sustainable and Integrated Energy Transition in Bavaria

Dr. Josef Hochhuber, Bayerisches Wirtschaftsministerium

9:45 – 11:00 a.m.

Energy Material Science: From Heat to Power to Building Applications

Session Chair: **Prof. Peter Müller-Buschbaum**

Development of Salt Hydrate Mixtures for Low-Temperature Latent Heat Storage

Christoph Rathgeber, ZAE Bayern, Energy Storage

A Newly Developed Reference Electrode for In-Situ Impedance Measurements in Sodium-Ion Batteries

Fabian Linsenmann, Chair of Technical Electrochemistry, TUM

Potential Use of Thermo-Responsive Polymers as Smart Window Surface Coatings

Lucas Kreuzer, Chair of Functional Materials, TUM

11:00 – 11:30 a.m.

Poster Presentation and Coffee Break

11:30 – 12:45 p.m.

Future Fuels: Power-to-X

Session Chair: **Prof. Hartmut Spliethoff**

Piping Renewable Energy: Utilizing Methanogen and Organic Waste

Robert Bauer, Deggendorf Institute of Technology

A Comparison of the Energetic Efficiency of the Production of Polyoxymethylene Dimethyl Ethers and other E-Fuels

Yannic Tönges, Chair of Chemical Process Engineering, TUM

Economics of Reversible Power-to-Gas

Gunther Glenk, Chair of Controlling, TUM

12:45 – 2:00 p.m.

Poster Presentation and Lunch Break

Please register: <http://www.mse.tum.de>

2:00 – 2:30 a.m.

Keynote: Food and Energy – Approaches to a Holistic Vertical Farming Concept

Dr. Petra Liedl, Munich School of Engineering, TUM

2:30 – 3:20 p.m.

Urban Energy Modeling

Session Chair: **Dr. Petra Liedl**

Integrated Urban Energy Modeling: Coupling Urban Growth with Energy Demand

Anahi Molar-Cruz, Chair of Energy Efficient and Sustainable Energy Systems, TUM

Solar Activated Envelopes in District Context – Energy Modeling Tasks

Lea Bogischef, Junior Research Group Cleanvelope, TUM

3:20 – 3:45 p.m.

Poster Presentation and Coffee Break

3:45 – 5:30 p.m.

Trends in Regional Energy Systems: A Bavarian Perspective

Session Chair: **Prof. Thomas Hamacher**

Retrofit Hybridization of Geothermal Binary Cycles in Southern Germany

Davide Toselli, Center of Energy Technology ZET, University of Bayreuth

Assessing Middle and Low Voltage Grid Requirements in Bavaria for the Decades to Come

Luis Ramirez Camargo, Team Geoinformatics, Deggendorf Institute of Technology

Comparison of different development scenarios for the energy system of the TUM Campus Garching

Benedikt Schweiger, Chair of Energy Systems, TUM

How can Prosumer Provide Flexibility to the Local Energy System?

Babu Kumaran Nalini, Chair of Energy Economy and Application Technology, TUM

5:30 – 6:00 p.m.

Keynote: The Antinomies of Climate Policy

PD Dr. Jens Söntgen, WZU Augsburg

6:00 – 6:15 p.m.

Summary and Closing

6:15 – 8:00 p.m.

Poster and Presentation Award with Colloquium Dinner

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1. Oral Presentations

Development of salt hydrate mixtures for low-temperature latent heat storage

C. Rathgeber^a, H. Schmit^b, P. Hoock^c, S. Hiebler^d

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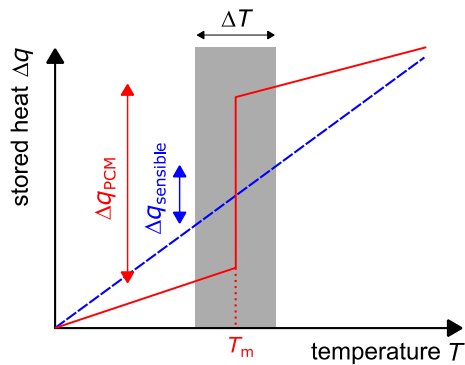


Figure 1: Latent heat storage compared with sensible heat storage

Latent heat storage using phase change materials (PCM) provides thermal energy storages with high storage capacities in small temperature ranges. Most of the PCM used in applications are solid-liquid PCM storing heat in repeated melting and crystallisation processes. Compared with sensible heat storage materials, e.g. water, an increased storage capacity can be achieved if both melting and crystallisation are within the range of charging and discharging temperature of the intended application. (Figure 1)

In the temperature range from 0 to 120 °C, salt hydrates are comparably cheap and offer high volumetric phase change enthalpies. However, in certain application-relevant temperature ranges, there is a lack of PCM based on salt hydrates that are cost-effective and thermally cycling stable. Since most salt hydrates are known, mixtures of salt hydrates are being investigated. In order to identify interesting compositions (e.g. ternary eutectics) and to reduce the experimental effort, thermodynamic prediction models are applied to calculate solid-liquid phase diagrams. The modified BET model requires only two model parameters and has proven to be able to predict phase diagrams of salt hydrate mixtures over a wide concentration and temperature range. The model parameters can be determined from the water activity of the binary subsystems which in turn can be calculated from water vapour pressure data.

In this work, a device for vapour pressure measurements of concentrated aqueous salt solutions has been constructed and applied to determine BET model parameters. Following this, ternary solid-liquid phase diagrams of systems containing water and salts with NO_3^- , Cl^- , Br^- , OH^- , and ClO_4^- as anions have been

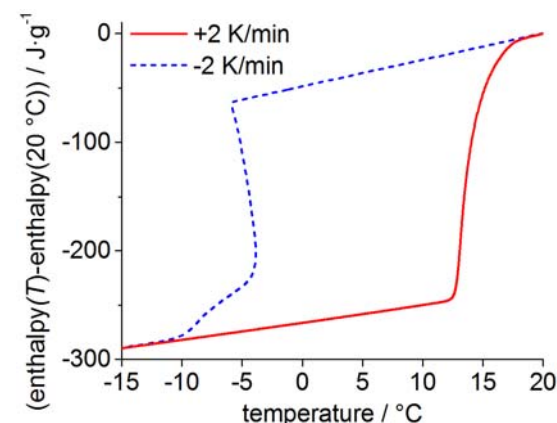


Figure 3: Enthalpy-temperature curves of the ternary eutectic within the system $\text{LiNO}_3 + \text{NH}_4\text{NO}_3 + \text{H}_2\text{O}$ measured via DSC

calculated using a self-programmed phase diagram prediction software on the basis of the modified BET model. (Figure 2) Thereby, ternary and pseudo-binary eutectics have been identified. In order to check the calculated phase diagrams, measurements via differential scanning calorimetry (DSC) of predicted eutectic compositions are being carried out. A single melting transition indicates a successful verification of the calculated eutectic composition (Figure 3). In addition, in order to improve the discussion of calorimetric results, crystallisation paths and corresponding enthalpy-temperature curves can be determined based on the calculated phase diagrams.

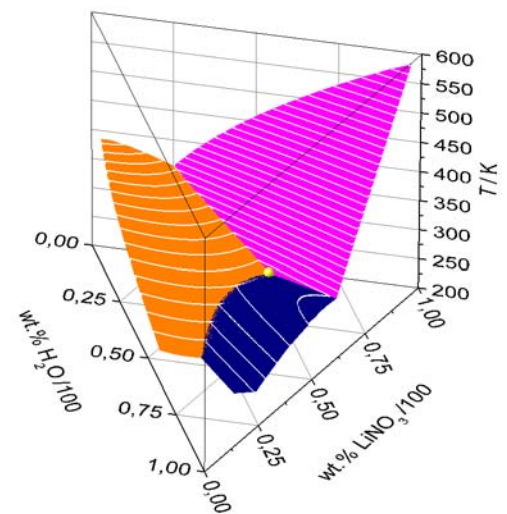


Figure 2: Solid-liquid phase diagram of the system $\text{LiNO}_3 + \text{NH}_4\text{NO}_3 + \text{H}_2\text{O}$ with ternary eutectic (yellow sphere)

A Novel Reference Electrode for Sodium Ion Batteries for in-situ Impedance Analysis

Fabian Linsenmann^a, Daniel Pritzl, Hubert A. Gasteiger

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Impedance measurements allow to gain valuable insights into resistances associated with intercalation phenomena of active species into electrode materials.[1] Monitoring changes of cell impedances during cycling can help identifying predominant ageing mechanisms responsible for capacity fading over the lifetime of a lithium-ion battery.[1,2] In order to differentiate between the contributions of anode and cathode to the full cell impedance, the measurement of symmetrical cells is commonly the most used method,[2] where two identical anodes or cathodes from aged cells have are harvested and reassembled in a new cell. State-of-charge (SOC) and/or state-of-life dependent analyses therefore require disassembly and reassembly of a large amount of cells. In order to measure anode and cathode impedance simultaneously, it is necessary to incorporate a reference electrode (RE) within the cell setup.[3] As shown by Solchenbach et al. for Lithium-ion Batteries (LIBs),[4] fundamental requirements for such a RE are that (a) its potential is stable within the measuring time of the impedance spectrum, (b) it is located centrally between anode and cathode, and (c) that its dimensions are small compared to the cross-sectional area of working (WE) and counter electrode (CE).

Within this study, we introduce a novel micro-reference electrode for Sodium-ion Batteries (SIBs) based on a sodium-tin alloy that is electrochemically formed in-situ after assembling the cell, further on referred to as Tin Wire Reference Electrode (TWRE). Hard carbons (HCs) are the most promising candidate anode materials for emerging SIBs.[5] With this RE we show SOC dependent impedance data of a SIB consisting of a commercial Hard Carbon (HC) anode and a Sodium Iron Phosphate (NFP) cathode. The NFP electrode was electrochemically prepared from a commercial Lithium Iron Phosphate (LFP) electrode via cation substitution.

We show that good impedance responses can be obtained in-situ by comparing the results with impedance measurements performed using the symmetrical cell approach. Figure 1 shows cathode and anode impedance spectra of an HC/NFP cell measured simultaneously at OCV directly after cell assembly using a TWRE. Furthermore, we will present impedance data from the first cycles of sodium intercalation into a HC anode, studying the SOC dependence of the charge transfer resistance (RCT) along with the formation of the solid electrolyte interface (SEI) and comparing it with impedance data from the literature obtained by symmetrical cells. These results will be contrasted with an analogous experiment where lithium is used as active species intercalating into the same hard carbon active material. The magnitude and the development of these cell resistances over cycling and implications on cell ageing and rate capability originating therefrom will be discussed.

Figure 1 shows the impedance spectrum for the NaFePO₄/HC full cell (red) together with the impedance responses of the HC anode (black) and the NaFePO₄ cathode (green) measured simultaneously.

The HC anode shows a transmission line like shape, whereas for the NaFePO₄ cathode at least two semi-circles can be identified. These features cannot be deconvoluted from the full cell spectrum.

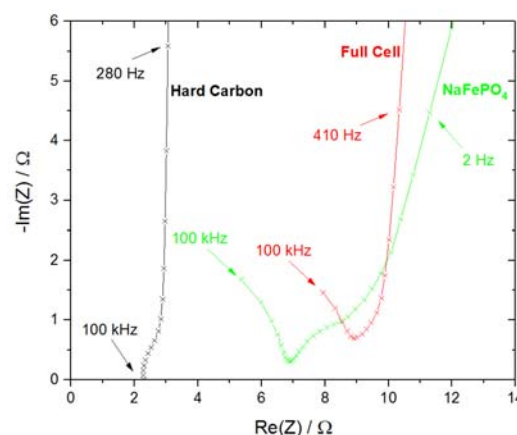
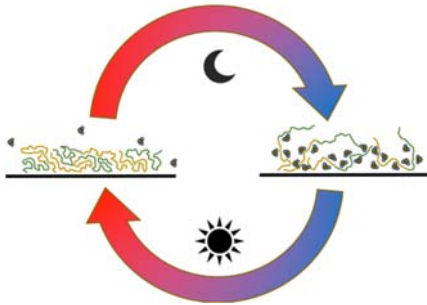


Figure 2: Cathode and anode-resolved Nyquist plots of a HC/NFP full cell measured at OCV after cell assembly. The impedance is recorded at 25 °C from 100 kHz to 1 Hz with a perturbation of 20 mV. The loading of the anode was 3 mgHC/cm² and 13 mgNFP/cm² for the cathode (0.95 cm² area each). A Swagelok-type 4-electrode cell with 60 μ l of 1 M NaPF₆ in EC/DEC (1/1 by volume) electrolyte and two glass fiber separators with a tin-wire reference electrode (TWRE) and a Na RE was used.

Potential use of thermo-responsive polymers as smart window surface coatings

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Today more than half of the world's population already lives in an urban environment and this trend will even increase to 70% by 2050 [1]. Therefore, a well-balanced energy management is necessary to keep the urban areas sustainable. In the United States over 40% of the energy consumption can be traced back to building utilities, of which cooling and heating are the main contributors [2]. Novel, ecological concepts for cooling have been proposed in the past years, mostly based on passive systems that are directly integrated in the roofs or the facades of the buildings. These systems demand autonomously adaption to fulfill the short-period need for cooling. Wet and/or cool conditions appear at least

once per day in most latitude areas and therefore cooling is only required between noon and midnight. A promising approach for self-cooling building is sweating. For example, mammals were able to live under environmental conditions of more than 25°C above their body temperature since they had the ability to sweat. With the transformation of this capability towards buildings an environmental friendly way of autonomous cooling can be achieved.

A simple and highly efficient way to cool buildings would be to use thermo-responsive polymer thin films as smart surface coatings since they undergo a phase transition either upon cooling (upper critical solution temperature – UCST) or heating (lower critical solution temperature - LCST). Above the UCST and below the LCST, polymer-solvent interactions are favored and H₂O molecules from the surrounding atmosphere diffuse into the polymer film. However, once the UCST is undershoot or the LCST is exceeded, respectively the polymer becomes more hydrophobic and water molecules are released out of the polymer film. The released water molecules evaporate and the building is cooled down by evaporative cooling. By combining both types of thermo-responsive polymers (UCST and LCST) a block copolymer with a highly tunable transition temperature is generated. In order to establish such thin polymer films in smart surface coatings a fundamental understanding in the kinetics is needed. Therefore, we investigate in-situ the temperature-dependent behavior as well as the reversible water storage/release of a poly(sulfobetaine) based block copolymer with neutron reflectometry in time-of-flight mode. With this sophisticated measurement technique, the kinetic processes can be followed with a high time-resolution and in great detail which results in a fundamental understanding of the underlying mechanisms of water uptake and release at different temperatures.

References

- [1] L. Cappelli, V. Guallart, Self Sufficient City, Iaa C-Institute for Advanced Architecture of Catalonia, Barcelona 2011
- [2] EIA, in Annual Energy Review, U.S.A. 2010
- [3] A. C. C. Rotzetter, C. M. Schumacher, S. B. Bubenhofer, R. N. Grass, L. C. Gerber, M. Zeltner, W. J. Stark, Adv. Mater. 2012.

Piping renewable energy: utilizing methanogen and organic waste

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Motivation

Sustainable energy supply today and in the future remains an intricate issue that calls for concerted political, technical and scientific efforts to overcome. One pressing aspect is the storage of renewable energy and the question how future transportation will be powered. One solution for both problems is chemical energy storage, namely methanation. Surplus renewable energy and CO₂ are hereby stored as bio-natural gas, which in turn can be fed into the gas network reducing the load on electrical grids. However, chemical processes demand rigorous conditions and are feasible only when using unpolluted gases due to the destructive influence of contaminants on catalysts.

Project and Technology

The biologic methanation of renewables has obvious advantages, first and foremost reaction speed of enzymatic catalyzed processes are much faster compared to chemical reactions. The catalyst is self-replenishing and therefore cheap. Another important factor are the moderate reaction conditions at 60 °C and about 3 bar for the biological methanation as compared to 250 – 700 °C and above 10 bar of pressure for the chemical process. Finally, methanogens can deal with syngas pollutants like H₂S, NH₃ or tar-byproducts very well and remove CO contamination completely, as already successfully shown during a preliminary study, namely “Ash-to-Gas”, conducted by a research associate and financially supported by the German Federal Ministry for Economic Affairs and Energy (Friedrich-Alexander-Universität Erlangen-Nürnberg 2018). Based on these facts a bio-natural gas plant is being constructed to test for efficiency and economic suitability. Combining hydrogen-rich gas from thermochemical biomass conversion with the electrolytic production of additional hydrogen with stoichiometric proportions to generate methane at a volume percentage of 96 or above, allowing to supply the gas grid (Fig. 1).

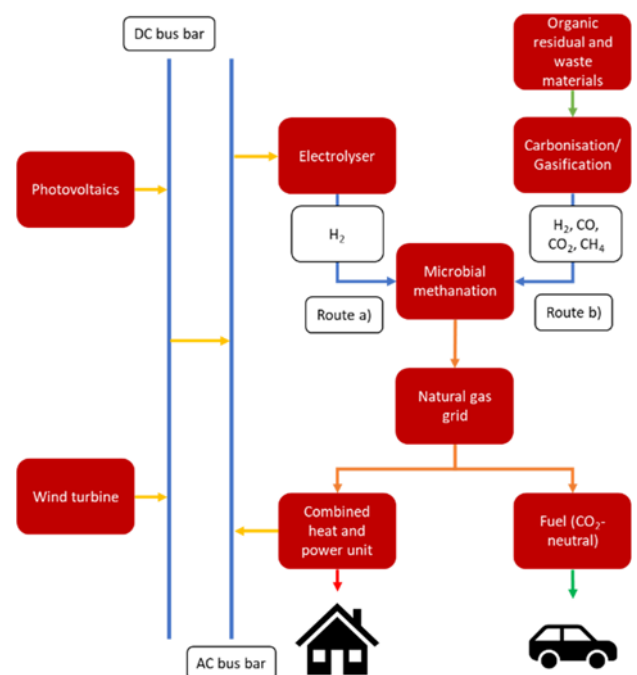


Figure 1: Chemical Storage Schematic for renewables: Route a) electrolysis, Route b) hydrogen-rich gases

Outlook

With the groundwork provided by this study industrial plants of adjusted size can be built in a demand driven manner at sites of surplus renewable energy, reducing the load of the electric grid. Further work building on the experience collected at the TZE can also establish whether modules of the plant may be operated at decentralized locations with, for instance, increased amounts of organic residue. By separating initial steps of the process some modules can be decentralized or even mobile. A prospected outcome is a centralized, industrial sized plant fine-tuned to maximize efficiency while small decentralized modules provide sufficient amounts of educts. This approach will contribute to sustainable energy supply for transportation, heating and electricity while simultaneously utilizing the energy contained within organic residue of various sources.

A comparison of the energetic efficiency of the production of polyoxymethylene dimethyl ethers and other e-fuels

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E-fuels produced from CO₂ and renewable energy have a high potential to reduce anthropogenic CO₂ emission in the future. Especially polyoxymethylene dimethyl ethers (OME) are highly discussed synthetic diesel fuels, they are organic compounds of the structure CH₃O(CH₂O)_nCH₃ (n = 3 – 5) which exhibit excellent fuel properties like high cetane numbers and soot-free combustion [1]. If OME are produced from renewable resources or CO₂, both via a syngas route, they will contribute to a significant reduction of overall CO₂ emissions [2]. This work presents results on the overall energetic efficiency of OME production when employing electrical energy and pure carbon dioxide as carbon source. In this work, the energetic efficiency is defined as the lower heating value of the OME fuel divided by the external energy input. The studied process chain consists of electrolysis for hydrogen generation, methanol production from carbon dioxide and hydrogen, an optimized formaldehyde process and two options to produce OME: A) a water-tolerant route in which methanol and formaldehyde are directly used as educts in OME synthesis [2], and B) a water-free route via methylal and trioxane [1]. The heat duties and their respective temperature levels along the route are collected from original process literature or estimated by process simulation in case of missing data. Pinch analysis is used to study various levels of heat integration. The influence of CO₂ capture is included in the analysis by considering direct air capture and post-combustion capture. The energetic efficiency of OME production is evaluated for 18 different scenarios (2 production routes, 3 levels of heat integration and 3 variants of CO₂ provision). A comparison of the current energetic efficiencies of the production of different e-fuels and the evaluation of maximum attainable efficiencies sets OME in an overall context and shows its high potential [3]. It is shown that the presented results hold qualitatively for all electrolysis efficiencies.

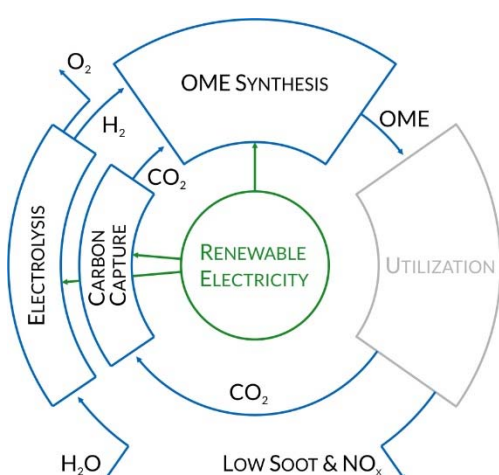


Figure 1: Graphical Abstract

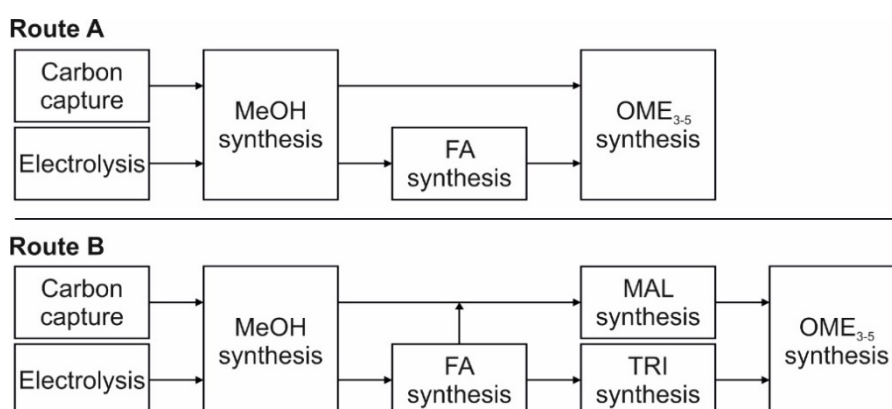


Figure 2: Two studied routes for the production of OME from CO₂ and water using electrical energy. Produced intermediates are hydrogen (H₂), methanol (MeOH), formaldehyde (FA), trioxane (TRI), and methylal (MAL).

- [1] a) J.O. Weidert, J. Burger, M. Renner, S. Blagov, H. Hasse, Ind. Eng. Chem. Res. 2017, 56, 575–582. b) T. Grützner, H. Hasse, N. Lang, M. Siegert, E. Ströfer, Chem. Eng. Sci. 2007, 62, 5613–5620. c) J. Burger, E. Ströfer, H. Hasse, Chem. Eng. Res. Des. 2013, 91, 2648–2662.
 [2] N. Schmitz, E. Ströfer, J. Burger, H. Hasse, Ind. Eng. Chem. Res. 2017, 56, 11519–11530.
 [3] M. Held, Y. Tönges, D. Pélerin, M. Härtl, G. Wachtmeister, J. Burger, Energy Environ. Sci.

Economics of Reversible Power-to-Gas

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The calculation of unit cost that can be used for estimating capacity investment decisions is frequently ambiguous due to the many ways to apportion applicable cash flows connected to the delivery of products. This paper studies the identification of relevant unit cost when productive capacity is shared among multiple outputs. Building upon the concept of levelized product cost, I find that unit cost should reflect a constant revenue payment required to break-even on the initial investment. This payment, which is shown to depend on the perspective that an investor can assume, determines the aggregation of upfront capacity expenditures with periodic operating expenses to the relevant cost and unit.

I apply the framework to examine new Power-to-Gas technology, which could become a central enabler of the transition towards a sustainable economy by reversibly converting electricity to hydrogen. Contrary to the common belief that fossil fuels are indispensable, my analysis shows that reversible Power-to-Gas will be sufficiently competitive with alternative fossil-based energy sources so as to provide a clean solution to the challenges of intermittent renewable electricity and widespread industrial decarbonization.

Integrated urban energy modeling: coupling urban growth with energy demand

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Our world is predominantly urban. Today, 55% of the total population lives in urban areas, a share that is expected to reach 68% by 2050 [1]. Cities are the main engines of the global economic growth as they concentrate industries, commerce, buildings and infrastructure. Urban inhabitants and their related activities consume around 75% of the global primary energy and are responsible for approximately 80% of the total greenhouse gas emissions [2]. As the world continues to urbanize, sustainable development depends increasingly on the successful management of cities, especially in low to middle-income countries where the fastest pace of urbanization is projected.

Cities are complex systems whose structure emerge from the bottom up. They are composed by autonomous agents that interact with each other and with their environment developing self-organizing adaptive systems. The resulting urban form and land use patterns affects the city's energy use and, consequently, the urban sustainability. Therefore, a comprehensive understanding of the relationship between the dynamic urban form and energy use is necessary for the formulation of effective policies towards energy-efficient and sustainable cities.

Cellular automata urban growth models have been developed and extensively adopted to study growth and expansion of cities. In this work, such a model is coupled with bottom-up energy demand models to first, understand the energy use patterns at the city level and, second, to estimate the future energy demand of an urban area. This integrated approach allows the inclusion of the –often ignored– spatially explicit urban transformations and expands the possibilities for incorporating other dynamic urban processes relevant for the shaping of a sustainable future (e.g. mobility and technology adoption).

[1] United Nations, Department of Economic and Social Affairs, Population Division (2018). World Urbanization Prospects: The 2018 Revision, Online Edition. Available at: <https://esa.un.org/unpd/wup/>.

[2] UN-Habitat, Urban themes: Energy, Online. Available at: <https://unhabitat.org/urban-themes/energy/>.

Solar activated envelopes in district context – energy modelling tasks

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The research project Cleanvelope aims to investigate how building envelopes can be energetically activated in terms of solar energy production. The focus is to show local and smart use of solar power including marketable interactions with the power grid and to identify the impact on urban microclimate.

An important aspect of the project is that the analysis of the energy system should be coherent with other project components including architectural and microclimate questions. A further challenge lies in including all relevant energy components of the district within one simulation model and at a suitable level of depth. This is important because by increasing the inflexible supply using solar power, the flexibility of other components becomes essential. This is where the load-shifting potential of a partially electrified heat and transport sector can play an important role and therefore needs to be included in the model.

To meet all of the criteria above, the model structure shown in fig. 1 has been developed. Weather data and information about the district in terms of building structure and user behaviour are inputs to the modelling elements. The next step is to derive the components for the optimisation from the input data. These include conventional electricity loads, electric vehicle loads, thermal loads, photovoltaic electricity production and any other supply and storage components. Furthermore, a holistic consideration should include the possibility of grid-supportive behaviour, which is realized via external price incentives. To identify optimal schedules for the flexible components a Model Predictive Control strategy is implemented which factors in predictions like weather forecasts. The optimisation identifies the most cost effective and energy efficient operational strategy, and provides schedules for all flexible components. In parallel to the optimisation, the influence of solar activated envelopes on outdoor comfort will be based on the same scenario input data. Grasshopper will be used as a platform to merge the different components of the analysis: it allows for data extraction from

3D-models and utilising the returned optimisation results for visualisation.

The aim of this approach is to deliver an energy model that is suitable for identifying the effect of solar activated facades in urban district context, using all options of flexibility within the system, and producing results that can be put together with architectural and microclimate investigations.

This project is sponsored by the Bavarian Ministry of Science and the Arts in the context of Bavarian Climate Research Network (bayklif).

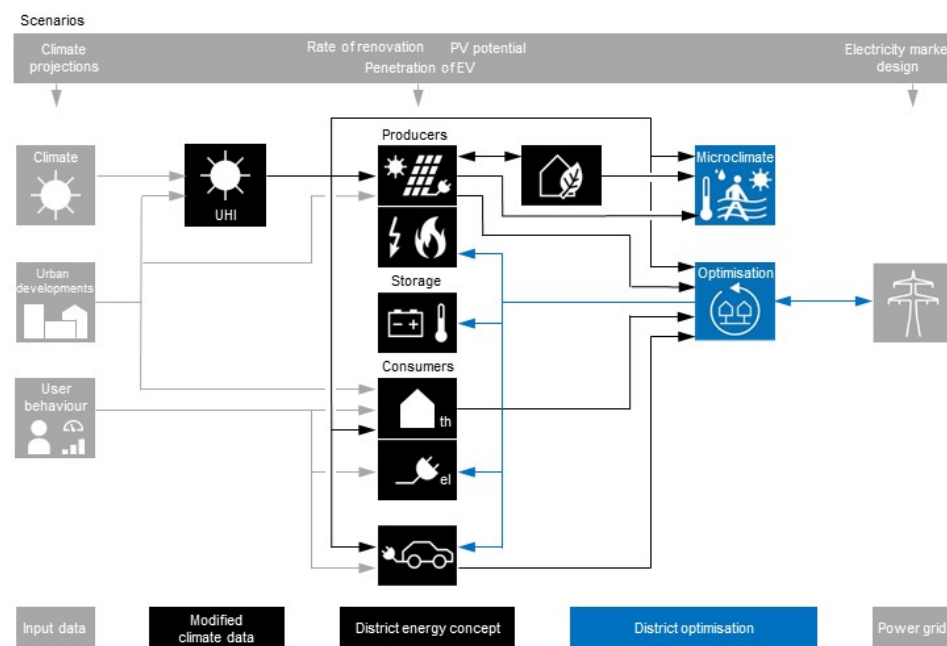


Figure 1: Model structure

Retrofit hybridization of geothermal binary cycles in Southern Germany

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Nowadays, the effects of climate change are increasingly encouraging the interest and developments of renewable sources.

Germany defined an ambitious social and economic plan in order to cut 80 % of CO₂ emissions by 2050. In this context, geothermal energy can play a significant role, since the high capacity factor and the possible CHP configuration. In Southern Germany, several power plants and district heating networks are running on geothermal energy. Coupling an existing geothermal power plant with a second additional renewable source can lead to significant improvements in annual energy production.

In this work, an Organic Rankine Cycle (ORC) geothermal system is modelled according to the properties of the geothermal reservoir in Oberhaching, Southern Germany. The on-design configuration of the system is performed as only geothermal exploitation. Later, a second renewable source is coupled to the existing system. Two different power plant layouts are investigated. In the former, the additional source is exploited in order to preheat the geothermal water before entering the ORC unit (Heberle et al. 2014). In the latter, the secondary source superheats the working fluid before entering the turbine (Heberle et al. 2017).

In particular, two different additional sources are investigated. First, biogas waste heat is recovered as additional renewable source in order to increase the ORC turbine power output (Toselli et al. 2018). In the most performing case study, the additional biogas thermal power (1350 kW_{th}) provides an increase of about +240 kW_{el} as turbine power output at 10 °C ambient temperature. An annual technical analysis is performed, providing +4.96 % increase in turbine power output. The low power output increase is limited by the low additional thermal power. Economic analysis suggests that a significant improvement can be reached only by reducing the cost of maintenance of the hybrid system. This assumption may reasonably derive from the close location of the two systems: the geothermal and the biogas one.

In order to augment the annual energy production, heat provided by the combustion of solid biomass is adopted as second renewable source. In this context, an available thermal power of 6000 kW_{th} provides an increase of +870 kW_{el} as turbine power output at 10°C ambient temperature. The overall annual energy increase results in +20.16 % on the simple geothermal system. Economic analysis highlights the importance of exploiting low-cost biomass, in order to maximize the feasibility of the retrofit. Next to power-only configurations, also CHP case studies are investigated. A real heat demand (Eller et al. 2019) is implemented in the models and techno-economic analyses are performed. The retrofit CHP configuration results slightly better than the retrofit power-only one, with a decrease of 0.47 €/ct/kWh as LCOE and 0.75 years as SPB.

References

- Eller, T., Heberle, F., Brüggemann, D., (2019): Transient simulation of geothermal combined heat and power generation for a resilient energetic and economic evaluation. In: *Energies*, March 2019 n. 12(5),894.
- Heberle, F., Brüggemann, D., (2014): Thermo-economic Analysis of Hybrid Power Plant Concepts for Geothermal Combined Heat and Power Generation. In: *Energies* n. 7, 7, pp. 4482–4497. DOI: 10.3390/en7074482.
- Heberle, F., Hofer, M., Ürlings, N., Schröder, H., Anderlohr, T., Brüggemann, D., (2017): Techno-economic analysis of a solar thermal retrofit for an air-cooled geothermal Organic Rankine Cycle power plant. In: *Renewable Energy*, 113, pp. 494–502. DOI: 10.1016/j.renene.2017.06.031.
- Toselli, D., Heberle, F., Brüggemann, D., (2018): Technical and thermodynamic evaluation of hybrid binary cycles with geothermal energy and biomass. In: Riehl, R., Preißinger, M., Eames, I., Tierney, M.,: *Proceedings of the Heat Powered Cycles Conference 2018*, pp. 443-450. Heat Powered Cycles. Bayreuth, Germany, 16.09.2018.

Assessing middle and low voltage grid requirements in Bavaria for the decades to come

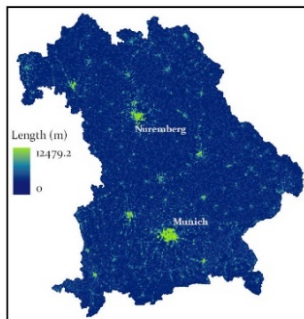
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Increased urbanization and rural depopulation processes are going to produce a high impact on the future electric grid. The impact of these developments on the shape and characteristics of the electricity transmission and distribution systems is however today not discussed as much as the transition to renewable energies. Current research dedicated to electrical grids focuses on the integration of renewables and the related necessary measures to increase stability and reliability. Topics such as the changes in the shape and length of grid as well as redundant infrastructure issues due to demographic changes are barely studied in previous literature. The present work is a pioneer attempt to address these issues using a spatially explicit approach for the state of Bavaria in Germany.

The main consequence emerging from depopulation is not only the increase on size and number of very low populated regions but also growing city-sizes, which up to now already have difficulties of being supplied with sufficient energy. Especially the difference in needs for the electricity grid length per person is going to be even more pronounced than already today. The resulting costs per person to provide everyone with a reliable electricity supply will diverge similarly between urbanized and rural regions. The medium and low voltage grids should be capable of delivering sufficient electricity to users and simultaneously allow the integration of distributed renewable generation installations. While data for analysing the transmission systems (high voltage grids) are widely available, spatial and attribute data of the medium and mainly the low voltage grids are scarce. The first step for the analysis of urbanization and rural depopulation effects on the future Bavarian low and medium voltage grid therefore is the estimation of today's electric grid.

Grid Length per km²

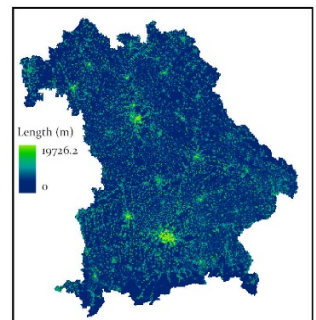


The present study proposes a method that relies on a) a data set that estimates the topology of the medium and low voltage grids of Bavaria (Germany) based on a minimum spanning tree principle, and b) data from the LUISA territorial modelling platform of the European Commission to calculate grid requirements for the years 2030 and 2050. Two alternative paths are proposed to carry out grid requirement estimations. The first is based on population data and the second on land use data. Grid length typologies are created based on population thresholds or land use types for 2010. The same typologies are afterwards used to extrapolate grid requirements for the future, which follow the population and land use changes of the LUISA data set. The future estimations are therefore in conformity with the forecasts utilized by the European Commission. As a reference base map for

comparing grid estimations based on population or land use clusters, the length of the grid calculated based on a) is cumulated for each square kilometer so that the resolution and extend match the LUISA data for Bavaria (the map on the left is the reference map for the medium voltage grid).

Results show that when estimating the current electricity grid based on land use clustering, it is not possible to get close to the beforehand calculated reference map. Using population density clusters on the other hand, makes it feasible to estimate the current electric grid based on mean or median grid lengths per cluster category. When comparing statistics as well as the resulting maps, the best method to produce a grid map based on clusters, is when using the median grid length per population cluster category (e.g. map on the right for the medium voltage grid). When using the mean of each category, the results seem not to be as precise. In the particular case of Bavaria, the forecast shows that total grid length requirements will decrease until 2030 and 2050. In rather urbanized regions, the grid needs to be prepared for expansions, while in rural regions existent grid infrastructure will become unnecessary. Hot-spots of such changes can be located using the results of the presented methodology.

Grid Length per km² (Median)



Comparison of different development scenarios for the energy system of the TUM Campus Garching

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The aim of this study is to compare different energy development scenarios for the TUM Campus Garching with regard to the greenhouse gas emissions and the economical costs until 2040. Effects of individual measures, e.g. the installation of photovoltaics (PV) or the decrease of the temperatures of the existing district heating network, on the energy supply system are evaluated.

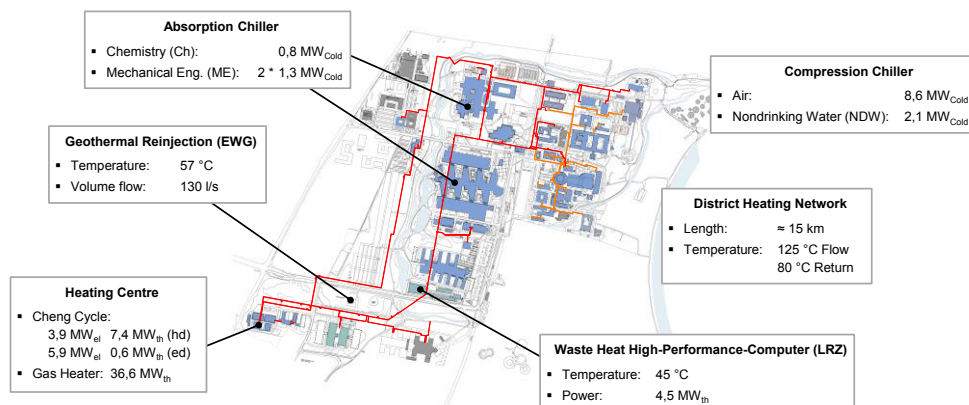


Figure 1: Current Energy Supply System of the TUM Campus in Garching

Based on forecasts of the electricity, heat and cold demand, the considered energy system is economically optimized for the timeframe from 2017 until 2044. Additional to the installed technologies (see figure 1) are about 15 different energy supply technologies and ten storage technologies to choose from. The development scenarios differ amongst other framework conditions in limits of CO₂ emissions, the biomass and biomethane potential, the time course and level of the temperature decrease of the heating network and the remaining term of the installed Cheng Cycle.

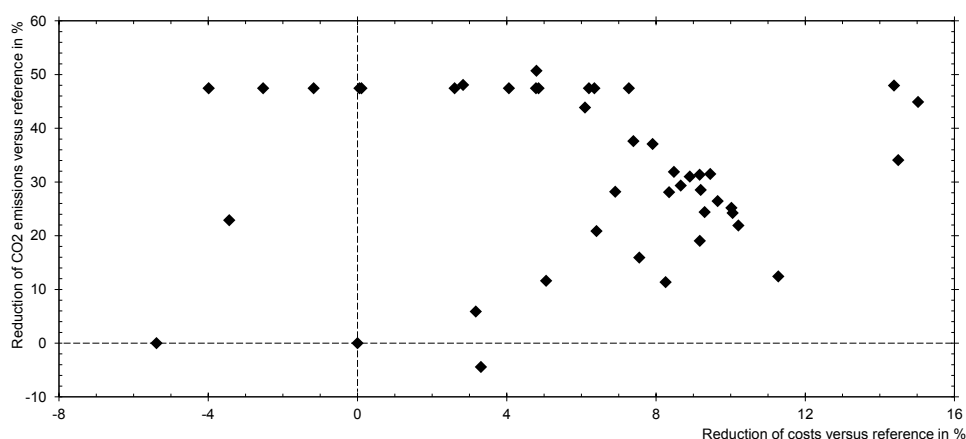


Figure 2: CO₂ emissions and costs for different development scenarios compared to the current energy system

Compared to the current energy system, both CO₂ emissions and costs can be reduced for most of the various scenarios (see figure 2). To achieve the CO₂ emission goals of the German government (until 2040 -55 % compared to 1990) for the TUM Campus in an economic way, two of the most effective measures are the reduction of temperatures of the district heating network and the installation of PV on the roofs.

How can Prosumer Provide Flexibility to the Local Energy System?

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With an increasing share of renewable energies and small-scale systems contributing to satisfy the load demand these participants in the electric system will also have to provide ancillary services as congestion management or operating reserve to ensure a stable and secure operation of power grids. A flexible operation of energy systems on a prosumer scale is required.

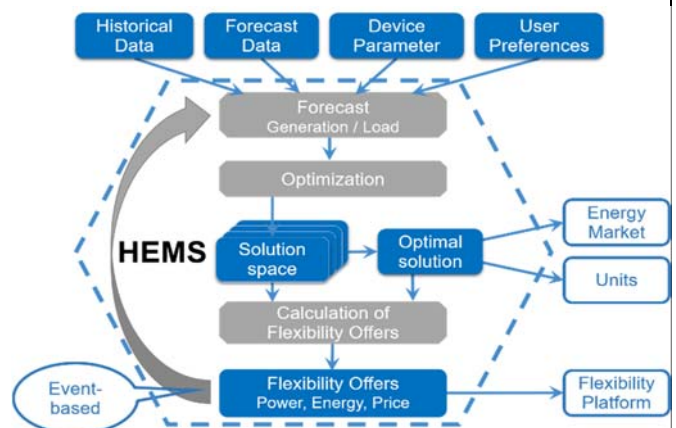
In this context the term “flexibility” comprises measures that influence the generation and/or consumption of electricity in reaction to an external signal (price signal or activation). Parameters as available amplitude of power modulation, duration, response time, location and price are used to characterize flexibility. [1]

“Prosumer” refers to consumers of electricity that generate part of their demand on-site and/or are able to influence their demand pattern actively. An energy management system (EMS) controls and optimizes the operation of the different energetic systems of the prosumer.

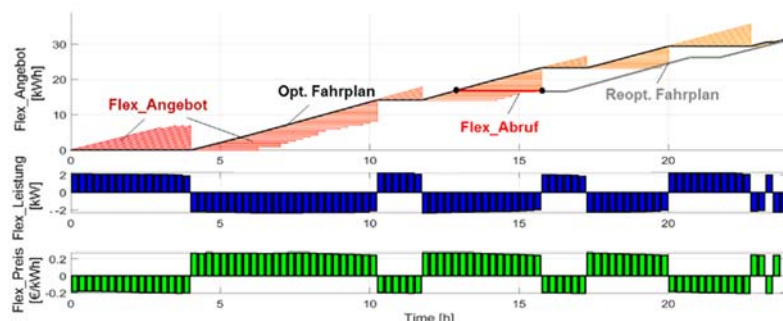
While energy is traded on energy market platforms, flexibility platforms are used to offer flexibility to grid operators. A communication infrastructure (ICT) connects prosumers and platforms.

In the following an approach to quantify and price flexibility provided by a prosumer is shown (figure below):

1. EMS generates schedules for the optimal operation of all relevant components based on prognosis of energy demand, availability of renewable resources and energy prices.
2. For each component that can be influenced, flexibility is determined as possible deviation from the optimal operation schedule. Power (kW) and amount of energy (kWh) is calculated.
3. For each possible flexibility, the additional costs for deviation from the optimal operation schedule are determined (€/kWh).



The figure below shows an example for optimal scheduling and flexibility offers of a heat pump. A negative price indicates that the prosumer benefits from operation of the heat pump during a call of flexibility and therefore is willing to pay for it.



Literature

- [1] D. Treballe und R. Otter, „Flexibility and Aggregation,“ 2014. Available: <https://www.usef.energy/app/uploads/2016/12/EURELECTRIC-Flexibility-and-Aggregation-jan-2014.pdf>. (accessed on 16 9 2018).
- [2] Zadé, Michel; Incedag, Yasin; El-Baz, Wessam; Tzscheuschler, Peter; Wagner, Ulrich, „Prosumer Integration in Flexibility Markets: A Bid Development and Pricing Model“ 2018. In: IEEE Conference on Energy Internet and Energy System Integration; Beijing Oct. 2018

Time	Power_scheduled [kW]	PosFlexPower [kW]	NegFlexPower [kW]	PosFlexEnergy [kWh]	NegFlexEnergy [kWh]	PosFlexPrice [€/kWh]	NegFlexPrice [€/kWh]
01.01.2019 03:30	0.000	1.980	0.000	1.046	0.000	-0.206	0.000
01.01.2019 03:45	0.000	1.864	0.000	0.519	0.000	-0.208	0.000
01.01.2019 04:00	2.185	0.000	-2.185	0.000	-4.881	0.000	0.265
01.01.2019 04:15	2.188	0.000	-2.188	0.000	-4.372	0.000	0.262
01.01.2019 04:30	2.225	0.000	-2.225	0.000	-5.559	0.000	0.268

2. Posters

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

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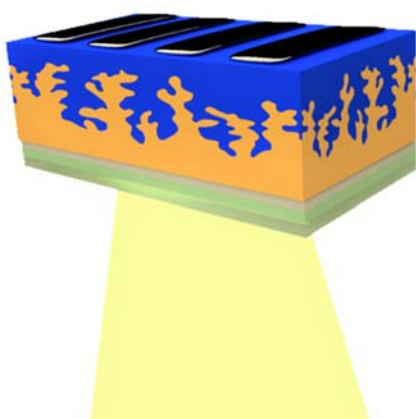


Figure 1: Device structure of an organic solar cell

Organic solar cells (Figure 1) offer several potential advantages compared to conventional silicon solar cells e.g. low weight, high flexibility and semi-transparency. This opens new fields of application e.g. solar windows, roofs and clothes.

Before commercialization, the fabrication process has to be up-scaled. Printing of active layers of organic solar cells with a slot-die coater might overcome this challenge. However, the morphology formation of printed organic photovoltaics has to be controlled to improve the solar cell performance.

The high-efficiency polymer PBDB-T-SF and the non-fullerene small molecule acceptor IT-4F which can reach a power conversion efficiency of 13 % [1] are printed out of chloro-benzene with a meniscus guided slot-die coater.

Grazing incidence small angle X-ray scattering (GISAXS) allows following the structure formation in situ during printing (Figure 2). This scattering technique provides fundamental knowledge to better understand the drying kinetics and morphology formation mechanism during slot-die coating of active layers for application in organic solar cells. In situ optical microscopy and UV/Vis spectroscopy were performed during printing to support the findings obtained from the scattering experiment.

Characterization techniques such as, photoluminescence and scanning electron microscopy (SEM) are applied after printing to get a deeper insight into the composition and morphology of the active layer of the printed films with the aim to further improve the solar cell efficiencies.

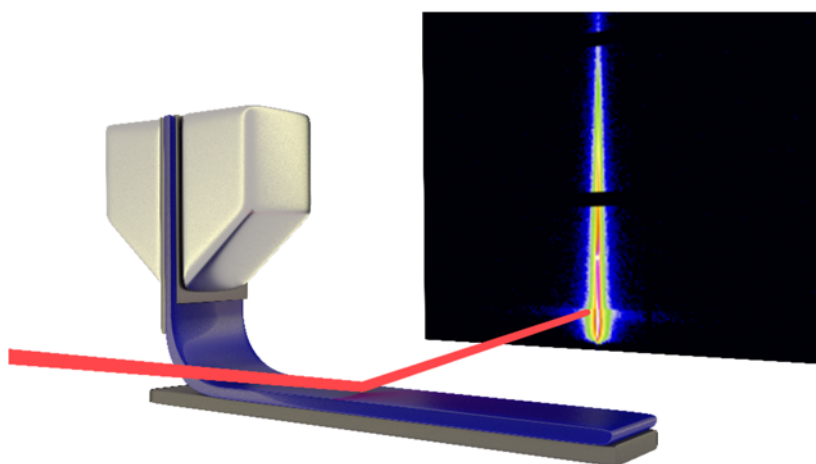


Figure 2: In situ GISAXS during printing of active layers based on the polymer PBDB-T-SF and the non-fullerene acceptor molecule IT-4F

References:

[1] W. Zhao, S. Li, H. Yao, S. Zhang, Y. Zhang, B. Yang, J. Hou J. Am. Chem. Soc. 139, 7148-7151 (2017)

Solar cell aging on a nanoscale – why even small changes can hurt

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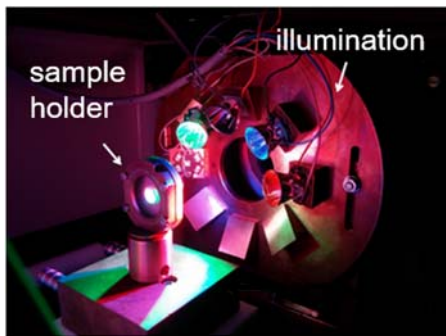


Figure 1: Illumination setup used to induce aging in photoactive thin films

With a growing population and an increasing living standard, the world's demand for sustainable energy is rising. Alternative energy sources such as solar, wind or hydropower already contribute significantly to the energy landscape in Germany with around 36.2 % of the overall produced electricity for 2017 [1]. However, they are typically limited to static, large-scale applications. Organic photovoltaics (OPV) have received high attention in recent years as an interesting alternative to conventional solar cells. Using polymer films as active material for energy conversion has a variety of potential advantages. Photoactive polymers can be synthesized from low-cost, abundant precursor materials and enable the formation of thin, light-weight and flexible films with tunable color. The devices can be produced via roll-to-roll processing, an easily up-scalable and thereby low-cost production technique. Due to these advantages, OPV devices could be integrated into a wide range of applications, combining functionality with design in fields as diverse as mobility, architecture or clothing.

Recent research efforts focus on enhancing the photovoltaic performance in order to make organic solar cells feasible for industrial purposes. This has led to the development of low band-gap materials with reported power conversion efficiencies nearing 12 %. [2] However, especially high-efficiency polymers are sensitive to various degradation processes, which strongly decrease their lifetime in comparison to commercially available inorganic photovoltaics. Several issues concerning the optimal thin film morphology and architecture will need to be addressed to make organic solar cells a potential candidate for mass market applications. Our work takes a deeper look at these aging processes of photoactive materials used in OPV devices.

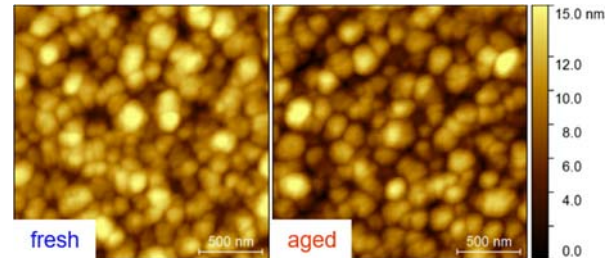


Figure 2: Microscopy images of a freshly prepared vs. an aged polymer film

We follow the chemical and physical changes occurring in low bandgap polymers during light-induced aging and test ways to eliminate typical degradation pathways. The thin film morphology is investigated using real-space imaging as well as X-ray scattering techniques. Optical and IR spectroscopy methods give insights into the chemical changes inside the polymer.

References

- [1] Quartalsbericht 04/2017, Umweltbundesamt, AGEE-Stat.
- [2] J. Zhao, et al., Nat. Energy 1, 15027 (2016)

Printing water-processed thin films for hybrid photovoltaic applications

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Due to the growing worldwide energy consumption, the use of solar energy as an abundant, clean and renewable resource is extremely attractive. The use of photovoltaic devices, which convert solar energy directly into electricity, has grown exponentially in the last decades and it is expected that it will continue growing in the next years. For this reason, innovative research in solar energy conversion is of fundamental importance. Silicon solar cells, with high conversion efficiencies, have been since many decades well established in the market. However, Si solar panels have many drawbacks such as being rigid, fragile, heavy and non-transparent. For this reason the so-called second and third generation solar cells have been developed.

Among these next generation solar cells we find hybrid solar cells, which aim to combine the advantages of both, inorganic and organic materials in the active layer. The stability and high carrier mobility of the inorganic component, together with the potential low-cost production and feasibility of producing flexible devices from the organic component make the hybrid approach promising. In particular, the possibility for wet chemical device preparation in the organic material allows the use of scalable thin film coating techniques. Most of the research in this direction use organic solvents for the solar cell preparation, which does not lead to a full environmentally friendly approach. Therefore, the use of water soluble components for the organic material is of interest. Slot die coating is a well-established technique in the industry due the potential coating over large surfaces, the possibility to coat at high speeds, little material waste in the overall process and the ability to integrate it in roll-to-roll systems. In the present study, we produce active layers from the following organic-inorganic components: a water-soluble polymer poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) and laser-ablated titania nanoparticles (TiO₂) fully processed in water. The active layer is deposited via slot die coating with a printing device built in our group. The investigation of the mesoscale structure and of the crystal structure is carried out via the scattering techniques GISAXS and GIWAXS, respectively, while UV/vis measurements are performed to study the absorption properties. To study the applications of this system, photovoltaic devices are built and its performance is studied.

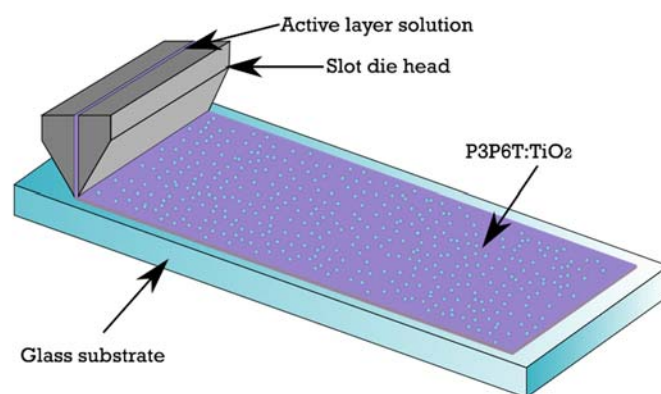


Figure 1: slot die coating of the active layer, showing the polymer (violet) and the TiO₂ nanoparticles (blue).

[1] K. Yoshikawa et al., Nat. Energy 2, 17032 (2017)

Functionalized silicon nanocrystals as active material in hybrid organic/ inorganic LEDs

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Organic light emitting diodes (OLEDs) are in mass production already with lower power consumption as conventional LEDs, but there is still room for improvement. One approach to improve LEDs is the usage of nanocrystals which show narrow emission spectra combined with potentially flexibility. The drawback of the commonly used II-VI and IV-VI nanocrystals is that they are based on Cd or Pb, for example, CdSe and PbS and therefore they are toxic. Silicon as bulk material is not suitable for LEDs due to its indirect bandgap. While shrinking silicon below the Bohr radius, the silicon nanocrystals (SiNCs) form a quasi-direct band gap and show strong photoluminescence. By varying the size of the SiNCs or the functional surface groups, the photoluminescence can be tuned across the visible spectrum. [1, 2] In this study, we keep the nanocrystal diameter constant and focus on the surface groups. The most common functionalization method for SiNCs is hydrosilylation (HS). Angi et al. compared the HS method with a novel organolithium method (OLR), depicted in Fig 1 a), and achieved higher performance as for reference LEDs using the HS method. [3]. In this study we investigate the effect of different chain length on the SiNCs.

A typical SiNC-LED device structure is shown in Fig 1 b). As the substrate, an indium tin oxide (ITO) structures glass is used. The ITO acts as a transparent electrode while the next layer, PEDOT:PSS acts as a hole transport layer (HTL). PolyTPD has two functions, it is used as HTL and at the same time it confines charge carriers in the SiNC active layer. ZnO serves as an electron transport layer (ETL) and on top, the thermally evaporated Ca and Al electrodes are used to inject charge carriers into the LED. For encapsulation, a thin glass slide is glued on top of the LEDs. To investigate the performance of the SiNC-LEDs, the luminance and current density are measured while sweeping the applied voltage. Additionally, the external quantum efficiency (EQE) was calculated based on the luminance data assuming Lambertian emission by utilizing the peak emission of the spectra.

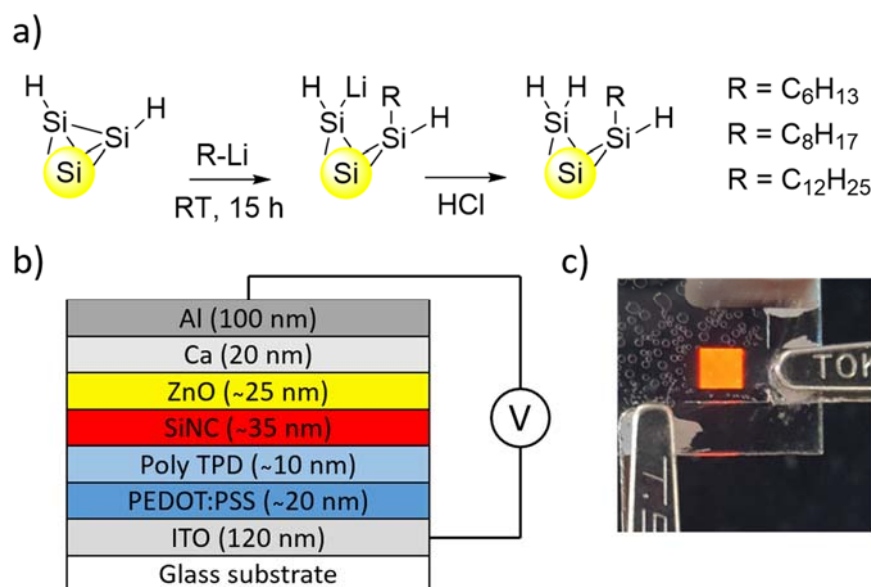


Figure 1: a) Schematic of the organolithium reaction method to functionalize the SiNC surface at a specific reaction temperature (RT). R represents the investigated chain length of C₆H₁₃, C₈H₁₇ and C₁₂H₂₅. b) LED stack with the corresponding film thicknesses. c) Picture of a SiNC-LED.

References:

- [1] D. P. Puzzo, et al., "Visible colloidal nanocrystal silicon light-emitting diode," *Nano Lett.*, vol. 11, no. 4, pp. 1585–1590, 2011.
- [2] M. Dasog, et al., "Size vs surface: tuning the photoluminescence of freestanding silicon nanocrystals across the visible spectrum via surface groups," *ACS Nano*, vol. 8, no. 9, pp. 9636–9648, 2014.
- [3] A. Angi, M. Loch, et al., "The influence of surface functionalization methods on the performance of silicon nanocrystal LEDs," *Nanoscale*, vol. 10, no. 22, pp. 10337–10342, 2018.

How to Choose an Interfacial Modifier for Organic Photovoltaics Using Simple Surface Energy Considerations

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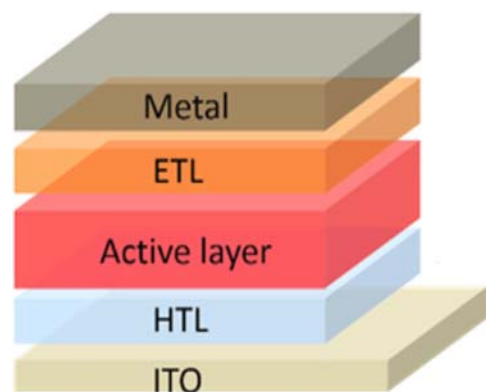


Figure 1: Structure of organic solar cell

Organic photovoltaics (OPV) are considered as one of the most potential alternative renewable and green energy sources due to the low cost, flexibility, solution processing and large-scale fabrication process. A typical OPV device comprises a layered structure in which a blend of donor and acceptor materials, the bulk heterojunction (BHJ), is sandwiched between the anode and cathode. Interfacial layers are employed in various locations within the sandwich architecture, notably between the BHJ and the electrodes to facilitate charge carrier collection. In the conventional forward structure (in Figure 1), the widely adopted configuration is ITO/PEDOT:PSS/BHJ/LiF/Al, which relies upon PEDOT:PSS and LiF as the key interfacial layers on either side of the BHJ. PEDOT:PSS has many known advantages, including high-conductivity, transparency, water-processability, and smoothing out the roughness of the underlying ITO.

However, the BHJ is a mixture of donor and acceptor polymers and/or small molecules, the accumulation of one of the components on the underlying electrode interface can be driven by surface energy considerations of the interfacial layer. A donor- or acceptor-rich interface may affect charge carrier flow to the electrode, thus affecting the overall efficiency. Therefore, efforts have been directed towards the development of PEDOT:PSS modifiers that modulate its surface chemistry. Here, ITO/PEDOT:PSS electrodes in forward OPV devices were treated with 5 thin interfacial layers (as shown in Figure 2) to change the relative surface energy of this electrode with respect to the adjacent BHJ. Based on the surface energies of polymers and interfacial modifiers, we describe a fast and straightforward approach to enable rational selection of an interfacial modifier on device performance, prior to device fabrication. By simply determining the surface energies of polymers and interfacial layers, the composition of the BHJ at the interfaces could be predicted, thus enabling the user to determine the effect, positive or negative, of the interfacial layer on the device performance. Predictions were confirmed by experimental characterization and device production and testing.

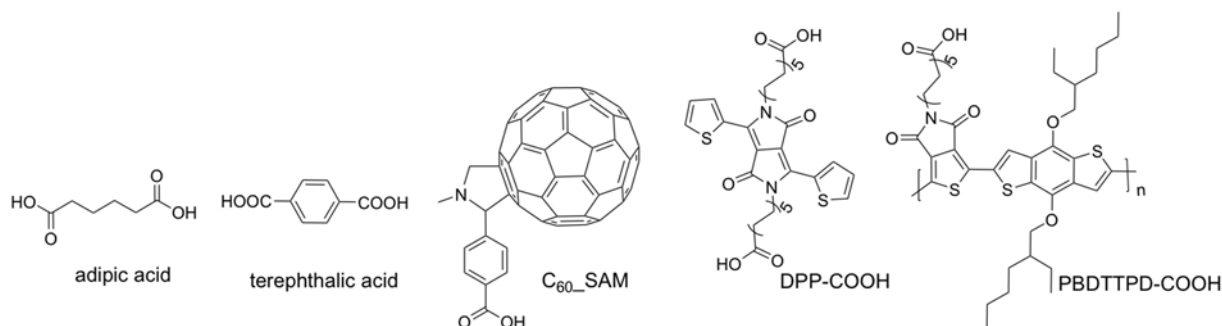


Figure 2. Chemical Structures of interfacial molecules and schematic of solar cell

In-Operando Observation for Performance of Perovskite Solar Cells under Light/Dark Cycling Condition

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The global energy demand is expected to increase significantly with the ever-increasing population, combined with industrialization and development. Fossil fuels are non-sustainable sources of energy and using fossil fuels also results in global warming. It is then, by all means, beneficial to switch over to renewable sources of energy like wind, solar, geothermal, hydroelectricity or biomass. Renewable energy also has the potential to help rural areas of developing countries, where it is much easier to generate energy locally from these renewable sources. Assuming a 20 % efficiency of solar cells receiving 1000 W/m² for 8 hours a day, the global energy consumption can be easily satisfied with just under 500,000 km² of solar panels based on currently available technologies easily. However, solar energy is still not widely adopted because of the higher cost per unit of electricity generated from solar panels. One of the main reasons for this is the high initial costs involved in fabricating ultra-pure silicon, which makes up most commercially available solar cells reaching up to efficiencies of above 20 %. For this reason, the different technologies of next generation thin film solar cells have emerged during last years. Several different technologies have emerged. Among these new technologies, mixed organic-inorganic hybrid perovskite solar cells have shown a promising future because of their outstanding photoelectric performance. Solution processing can be used to achieve low-cost manufacturing of these solar cells. The Power Conversion Efficiency (PCE) of Perovskite Solar Cells (PSCs) has been enhanced to 23.7 %¹, making this technique competitive with commercial silicon solar cells.

Despite all these advantages, the application of PSCs is currently limited by combining high performance and operational stability because PCE of PSCs can degrade under pressure of temperature, light, humidity and oxygen². In addition, the rapid developing progress in the fabrication of PSCs has not been accompanied by the development of start-of-the-art characterization methods. Current degradation researches on PSCs are performed by a simple current-voltage measurement. Therefore, it is necessary to introduce new characterization tools for analyzing degradation mechanisms of PSCs.

We propose to observe degradation process of PSCs under illumination condition through using in-situ grazing incidence wide-angle X-ray scattering (GIWAXS) and grazing incidence small angle X-ray scattering (GISAXS), aiming to acquire the evolution of structure and morphology under illumination. What's more, recently, there are researches showing reversible improvement and degradation of PSCs under illumination-darkness cycling³. GIWAXS and GISAXS would be a powerful tool to dig the mechanisms of the reversible improvement and degradation out. After understanding mechanisms behind, potential solutions could be found to suppress the degradation process of PSCs.

[1] NREL. Best Research-Cell Efficiency Chart, <<https://www.nrel.gov/pv/assets/pdfs/best-research-cell-efficiencies.pdf>> (2019).

[2] Berhe, T. A. et al. Organometal halide perovskite solar cells: degradation and stability. *Energy & Environmental Science* 9, 323-356 (2016).

[3] Domanski, K., Alharbi, E. A., Hagfeldt, A., Grätzel, M. & Tress, W. Systematic investigation of the impact of operation conditions on the degradation behaviour of perovskite solar cells. *Nature Energy* 3, 61 (2018).

In-situ investigation of sputter deposition electrodes for organic solar cells

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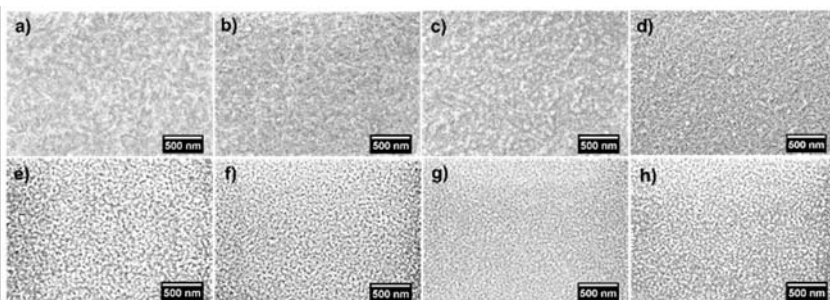


Figure 1: SEM images before(a-d) and after(e-h) Al deposition

Bulk heterojunction (BHJ) polymer solar cells have gained significant improvements via both novel organic synthesis and easy fabrication methods. Especially the fabrication through solution allows for large scale deposition processes such as roll to roll printing. Furthermore, the application of conjugated polymers as functional layers makes organic solar cells an attractive approach for a cost-effective solution to current energy-shortage issue. Recently, the efficiencies

of non-fullerene organic solar cells (OSCs) with small molecule acceptors rapidly increased to over 16%, which makes OSCs competitive to commercial available solid state solar cells [1]. However, in order to make OPVs commercial competitive on the long term, overcoming degradation and achieving long device's lifetime is of significant interest. The peeling-off of the electrode from the contact layer surface caused by aging stresses lead to an intrinsic degradation, which is one of the main reasons for performance loss of OSCs [2]. Although thermal evaporation technique is a common method of fabricating the electrode due to its low cost, this technique brings a number of problems for the device such as soft contact between electrode and function layer interface. Another disadvantage is inevitable high temperature during fabrication process. Sputter technique is a promising technique to solve these issues.

For understanding the mechanism of the metal cluster growth on the thin films with various morphology, we introduce in-situ grazing incidence small angle X-ray scattering (GISAXS) technique to observe the morphology change during sputter process. In-situ GISAXS measurements during sputter deposition of Al nanolayers are conducted at the beamline P03 of DESY in Hamburg via using a DC magnetron sputter chamber. Figure 1a-b show that active layers contain a PffDT4T-2OD donor with a small molecule acceptor EH-IDTBR blender dissolved in 1,2,4-trimethylbenzene and chlorobenzene respectively. Then 10nm MoO₃ blocking layers were deposited on their top surface, corresponding to Figure 1c-d. Figure 1e-h show the morphology of thin films after 20nm Al layer deposition through sputter technique. These SEM images indicate that the morphology impact on the Al growth significantly. The morphology evolution during Al nanolayers growth observed in the out-of-plane cuts as shown in Figure 2. All peaks of different thin films appear at lower δ . These peaks move from large to small q_y values with increasing δ , which can be assigned to Al particles and clusters appearing during the sputter process. It should be note that the formation of Al layers with one layer MoO₃ deposited on the active layer is slower than the active layer without deposition of MoO₃.

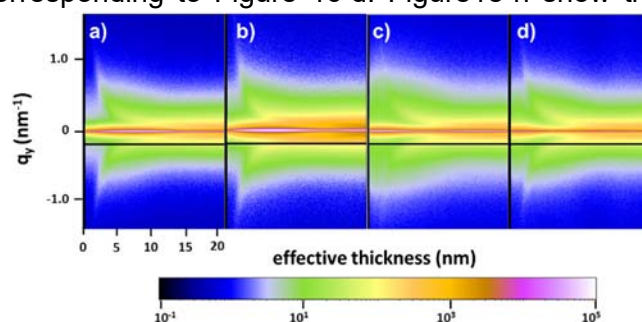


Figure 2: out-of-plane cuts q_y in the range of the Yoneda peaks versus the effective film thickness δ

[1] Fan B, Zhang D, Li M, Zhong W, Zeng Z, Ying L, et al. Achieving over 16% efficiency for single-junction organic solar cells. Science China Chemistry. 2019.

[2] Mateker WR, McGehee MD. Progress in Understanding Degradation Mechanisms and Improving Stability in Organic Photovoltaics. Advanced Materials. 2017;29(10):1603940.

Spray deposition of bio templated titania for hybrid solar cells

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Since the beginning of industrial age, humanity has an exponential growing demand of energy supply. The use of fossil fuels is not only restricted to a very limited amount of resources, it further also enhances climatic changes and has a strong impact on nature. Therefore, supplying clean, safe and renewable energy is an essential task. For the benefit of this, it is of reasonable interest to enable energy consumers satisfying their own demand based on renewable energy sources. Towards this self-sufficient and “green” energy supply,

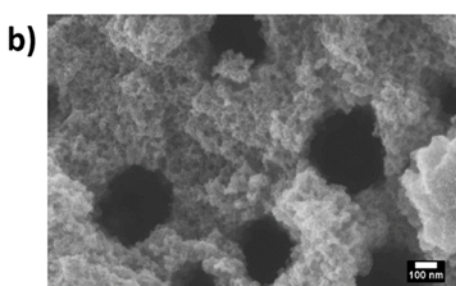
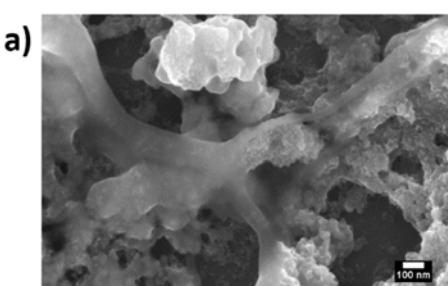


Figure 1: a) β -Lg:titania precursor composite b) hierarchical TiO_2 after calcination

the possibility of large scaled and cheap roll to roll solar cell fabrication based on organic materials is an important step. With the potential of flexible, semi-transparent properties these solar cells open new paths of design and application, for example integrated in architecture, clothing and all day accessories. Enhancement of these solar cell's lifetime and efficiency is a key challenge. Thus, we want to

combine long term stability and high charge carrier mobility with flexibility and large scale fabrication of inorganic and organic materials in hybrid solar cells (HSC).

For this purpose, nanostructured titanium dioxide films have great potential as the inorganic counterpart in these HSC. The film morphology has crucial influence on the device performance, since a high surface-to-volume ratio is needed for efficient charge separation. So far, inorganic mesoporous matrices are successfully achieved by sol-gel chemistry in combination with block copolymer directed templating. As a novel approach, we use environmentally friendly biopolymers as tailoring agents. The whey protein β -Lactoglobulin (β -Lg) was found to form different structures within denaturation, from fibrils to spheres [1]. By combining heat denaturation at different pH and sol-gel chemistry, different nanosized structures are introduced into titanium dioxide. The resulting sol-gels are used as inks for film deposition via spray coating. In situ grazing incidence small angle X-ray scattering (GISAXS) measurements display the complex morphology evolution during the spray coating process [2]. After calcination to remove the biopolymer template, the film morphologies of the remaining titanium dioxide scaffolds are investigated by GISAXS, which is further supplemented by scanning electron microscopy measurements.

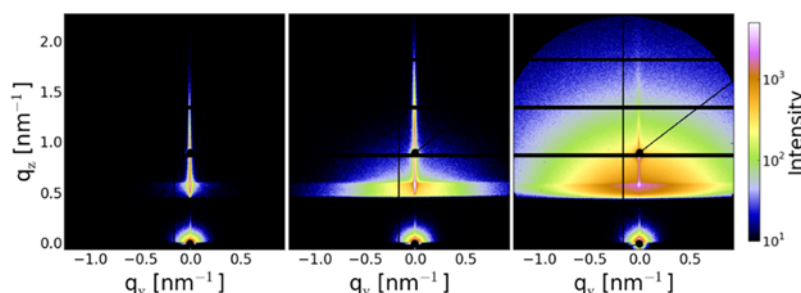


Figure 2: In situ GISAXS displays film evolution during spray coating

References

- [1] J.-M. Jung, et al.: “Structure of Heat-Induced β -Lactoglobulin Aggregates and their Complexes with Sodium-Dodecyl Sulfate”, *Biomacromolecules*, 2008, 9 (9), pp 2477–2486
- [2] N. Hohn, et al.: “Impact of Catalytic Additive on Spray Deposited and Nanoporous Titania Thin Films Observed via in situ X-Ray Scattering: Implications for Enhanced Photovoltaics”, *J. Phys.: ACS Appl. Nano Mater.*, 2018, 1 (8), pp 4227–4235

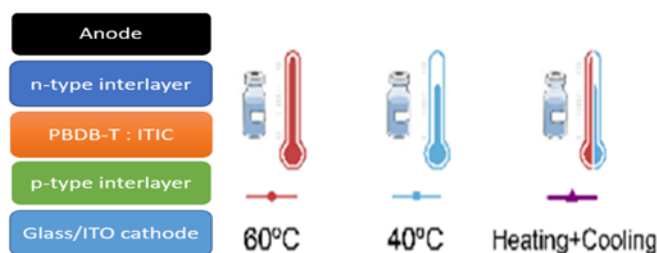
Influencing the properties of fullerene-free bulk heterojunction blends for photovoltaic applications

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As a technology for converting sunlight into electricity, organic solar cells (OSCs) have shown a great potential to be utilized for different applications due to the possibility to produce large areas at low cost and being environmentally friendly. An efficient way of converting the energy at OSCs is to use one donor and one acceptor in order to make a blend of polymers by controlling different parameters. Processing binary OSCs with fullerene-free acceptor material is of great importance, since it has provided further progress concerning higher power conversion efficiencies (PCE) [1]. One of the prerequisites of increasing the photon harvesting of active layers and thus obtaining highly efficient OSCs is differing the parameters of processing and adding additives to the blend of polymers [2]. The key role in influencing the properties and progress in the functionality of these polymers by changing the parameters can be due to the modification in the morphology. The morphology, which involves molecular orientation, crystallinity and aggregation of the polymer molecules, can be tuned with different techniques, such as solvent annealing, thermal annealing of the substrates with active layers and solvent additives.

The above mentioned methods of improving the morphology can be implemented during blending the solution of donor and acceptor. The polymers which are used in this work demonstrate the notable change in the absorption spectra at different temperatures. Aggregation of the molecules and intramolecular twisting can be a cause for this change in the absorption spectra. For understanding the effect of annealing and adding the dopants, the photoluminescence measurement (PL) and UV-Vis are performed for the blend solution and neat polymers spin-coated thin films.



The advantage of increasing and subsequent decreasing the temperature of the blend solution can be attributed to the increase in the absorption of the polymers and decrease in the PL intensity which is related to the mild aggregation and averaged molecular twisting by which the charge mobility and thus the PCE of OSCs can increase. Moreover, the importance of the subsequent cooling of the polymers blend in this work can be due to the recovery of the intermolecular twisting that was removed before by heating the blend. Therefore, better charge transfer can happen from the donor to the acceptor polymer. In addition to the annealing process of the blend of polymers, the incorporation of additives in the blend can have different influences on the resultant polymer blend which are regarded to the enhanced surface morphology and better aggregation with small size of the polymers. As the result, the additives can be a reason for higher exciton dissociation efficiency and improve in the energy conversion of the processed cells.

References

- [1] Shenkun Xie, Jianqiu Wang, Rong Wang, Dongyang Zhang, Huiqiong Zhou, Yuan Zhang, Defeng Zhou, Chinese Chemical Letters <https://doi.org/10.1016/j.ccllet.2018.04.001>
- [2] heng, Yifan. (2018). Materials Today. 21. 10.1016/j.mattod.2017.10.003.

Nanoscale crystallization of conjugated polymer PffBT4T-2OD in printed titania pores

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During the past decade, hybrid solar cells (HSCs) have received considerable attention for solar energy conversion because they possess the combined advantages of conjugated polymers and n-type inorganic semiconductors, such as low cost, ease of production and high efficiencies. Particularly, anatase titania, as an electron-transport material, has been widely studied, because it has a wide bandgap, high electron mobility and long charge-carrier lifetime. Recently, poly[(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3"-di(2-octyldodecyl) 2,2';5',2";5",2'''-quaterthiophen-5,5'''-diyl)] (PffBT4T-2OD), which yielding device efficiencies $\approx 11\%$ in a single junction organic photovoltaics, holds promising to achieve high efficiency in HSC application. Like in the organic photovoltaics, the bulk heterojunction concept can also be applied for HSCs. This means the control over morphology, crystallinity and the polymer chain orientation is of great importance for device performance. So far, the sol-gel chemistry combined with an amphiphilic block copolymer has been proven to be a promising route to tailor the nanostructures of TiO_2 films. However, the studies about the crystallization behavior of PffBT4T-2OD inside the TiO_2 pores are rare, in particular concerning large-scale deposition techniques.

In the present work, we use slot-die printing combined with wet chemistry to fabricate controllable mesoporous TiO_2 nanostructures in large scale. Subsequently, the mesoporous TiO_2 films with different pore size are backfilled with PffBT4T-2OD. TiO_2 film morphology is investigated by scanning electron microscopy (SEM) and grazing incidence small-angle X-ray scattering (GISAXS). Particularly, GISAXS reveals the sizes of the nanostructures and pores of the printed TiO_2 films. In order to investigate the effect of TiO_2 pore size on the crystalline properties of the conjugated polymers PffBT4T-2OD, e.g. lattice distance, crystal size or orientation, grazing incidence wide-angle X-ray scattering (GIWAXS) is applied to probe the hybrid films. PffBT4T-2OD crystals with a denser packing of polymer chains exist in the large pore size of TiO_2 films. Moreover, a high face-on to edge-on ratio also preferentially appears in the large TiO_2 pores.

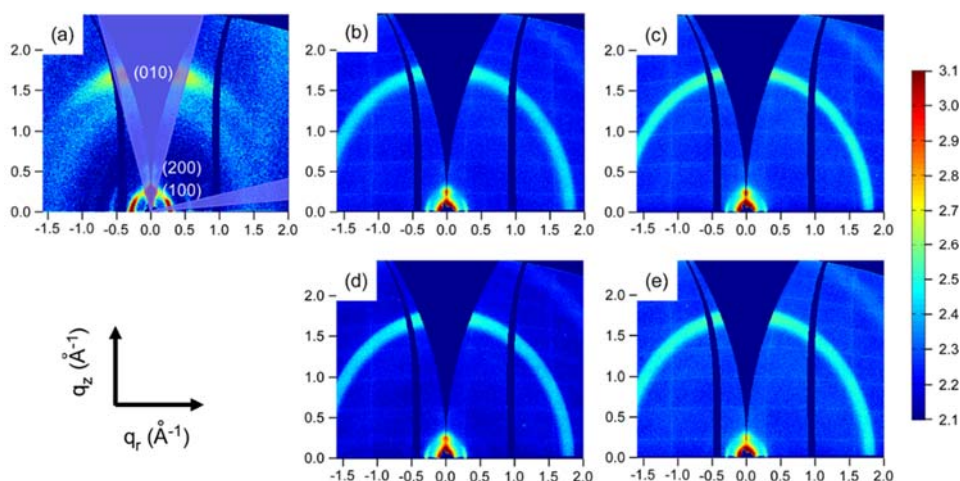


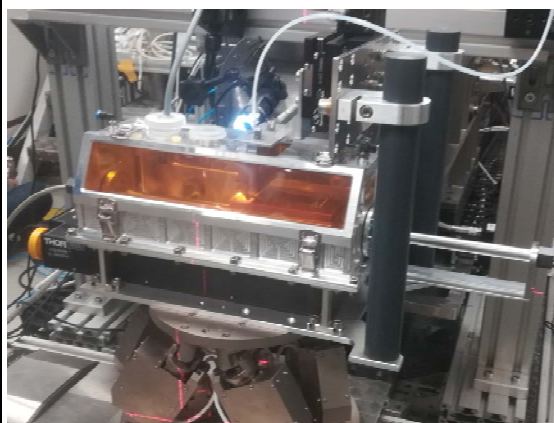
Figure 1: 2D GIWAXS data of (a) a pure PffBT4T-2OD reference sample and the printed mesoporous TiO_2 films backfilled with PffBT4T-2OD with varying weight fraction of TTIP: (b) 1.5%, (c) 2.0%, (d) 2.5% and (e) 3.0%.

Printing low-bandgap based bulk heterojunctions for photovoltaic applications

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The conversion of energy out of sunlight is an indisputable promising possibility to tackle the problem of continuously growing energy demand. Standard devices for light harvesting are commonly based on inorganic compounds like silicon or gallium arsenide. Over the last decades, organic photovoltaics have emerged as a promising alternative to replace the conventional solar cells, due to their advantageous characteristics, such as light weight, flexibility, and solution processability. Especially, since organic photovoltaics surpassed power conversion efficiencies of 11% [1], they have drawn attention in industry for commercialization. The possibility to process this kind of solar cells out of solution allows the usage of low-cost and less energy consuming manufacturing techniques, like roll-to-roll coating, spray casting or printing, which are large scale deposition methods and already well established in industry. The usage of such techniques not just reduces the production cost, but also the energy payback time of these devices.



Hence, taking the step towards large scale processing, the influence of the methods on the overall performance of photovoltaic applications have to be studied and understood. Since it is known, that the buried structure within the photoactive layer is an important key for an effective device performance, the influence of the printing process on the inner morphology of the photoactive thin film has to be investigated. Therefore, X-ray scattering techniques are suitable tools to probe not only the surface but also the inside of these layers. Furthermore, X-ray scattering techniques allows the monitoring of the printing process in-situ.

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

References

- [1] W. Zhao, D. Qian, S. Zhang, S. Li, O. Inganäs, F. Gao, J. Hou, Adv. Mater., 28, 4734 (2016)
- [2] A. Hexemer, P. Müller-Buschbaum, IUCrJ, 2, 106 (2015)

Printed Quantum Dot Solid for Photovoltaics

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Colloidal quantum dots (CQDs) have attracted many attentions for various electronic applications, like light emitting diodes, photodetectors, photovoltaics etc. due to their unique intrinsic properties, like tunable energy band-gap and stability against ambient circumstance. Comparing with cadmium chalcogenides CQDs, the lead chalcogenides CQDs reveal much weaker exciton binding energy because of the smaller effective electron mass, which is beneficial for the extraction of electrons and therefore suitable for being utilized in photovoltaics (PV) rather than light-emitting diodes.

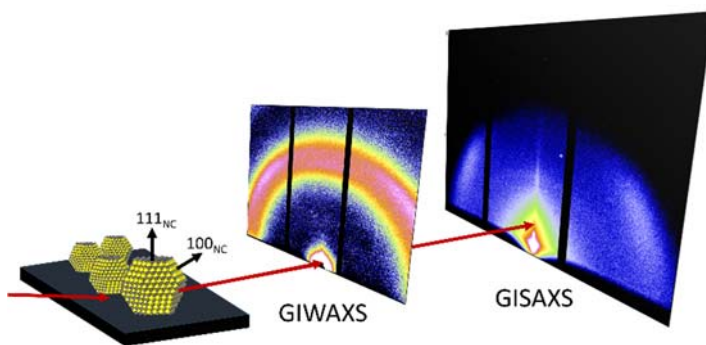


Figure 1: GIWAXS and GISAXS measurements on a CQDs' array solid. red arrows: incident and reflected x-ray

Size-monodisperse CQDs are normally obtained from a hot-ions injection method in solution. The long-chain organic ligands, like oleic acid chains, are necessary to be employed as surface surfactants to prevent the CQD's aggregation during the fabrication process, purification process and long-time storage afterwards. In order to realize and improve the charge transportation among CQDs' array, the distance between each CQD is required to be decreased reaching a certain value homogeneously. The long chain ligands are always removed during the ligand exchange process and film deposition. Thus, the wavefunction of as generated excitons could have larger overlap and

better electronic coupling for forming energy transport tunnels.

In this work, the ligand exchange process of CQDs have been carried out in a solution phase by various chemical treatments, including Methylammonium Iodide (MAI) in N,N-Dimethylformamid (DMF) as one of the recipes. The ligand-exchanged CQDs were obtained after several washing processes and then re-dispersed in octane. For device fabrication, we selected conventional ITO as the conductive substrate and ZnO was formed as the electron transport layer (ETL) through a sol-gel method. The ligand-exchanged CQDs were printed on the ETL directly to form an active layer. Then 1,2-Ethanedithiol (EDT) treated CQD layer was coated on the active layer to act as an electron blocking layer. Gold was finally deposited on the top of the device as electrodes by vacuum evaporation. We used grazing incidence small angle / wide-angle x-ray scattering (GISAXS/ GIWAXS) to investigate the inner structure of the active layer.

Our results indicate that different chemicals for ligand exchange process of CQDs lead different inner structure of the active layer, which has been confirmed from our GISAXS/GIWAXS results. The correspondent device performances based on different active layer have been also discussed.

Following the interface formation during gold sputter deposition on perovskite films

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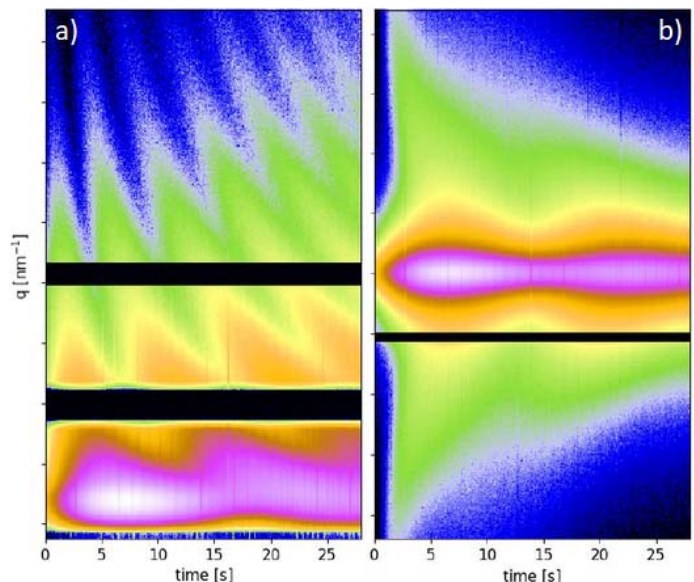
Currently, humanity is approaching an age of global warming due to the unsustainable consumption of fossil fuels. Considering also the continuously growing global power demand, a quick change towards clean and renewable energy production is therefore essential. Sunlight is one of the most promising energy source and already used successfully in silicon-based solar cells (SCs) to produce electric power. However, their resource- and energy-intensive and therefore cost-intensive production drives the search for novel material based thin-film SCs, which are a promising alternative to silicon-based SCs in the near future.

Recently of special interest are perovskite SCs with their impressive increase in efficiency over the last years to more than 22 per cent – promising for future and sustainable power production [1].

Perovskite thin films with high quality crystals are produced easily at low temperatures in the lab-scale spin-coating process, but could be processed equally well in up-scalable industrial deposition techniques as printing or spray casting.

In the industrial production of SCs, also sputtering is a common technique to deposit metal electrodes of nanometer thickness on the thin film because it is well-controllable and cost-effective process. In addition, sputtering preserves the layer beneath it, compared to chemical or thermal deposition techniques. Understanding and controlling the interface formation during the sputtering process is therefore important to develop highly efficient devices, not only SCs but also phototransistors as well [2].

In the present study, perovskite (methylammonium-lead-iodide, MAPbI₃) thin films were deposited onto silicon substrates via spin-coating and subsequent annealing. During the gold sputter deposition, in-situ grazing incidence small angle X-ray scattering (GISAXS) was performed to gain insight into the detailed steps of aggregation and growth of the sputtered metal layer [3]. Thereby, GISAXS offers a nondestructive way to gain information of high statistical relevance about the time evolution during the crucial steps of interface formation. The focus in the analysis of the resulting in-situ data is on the Yoneda region – characteristic for every material – containing the desired information of the bulk and surface morphology in reciprocal space. To access this information, horizontal line cuts reveal details of the lateral formation of the gold clusters, i.e. parallel to the surface. This allows following the process and different stages of growth and clustering of the metal grains until the interface formation is complete.



- [1] M. Saliba, J.-P. Correa-Baena, C. M. Wolff, M. Stolterfoht, N. Phung, S. Albrecht, D. Neher, A. Abate, *Chem. Mater.* **30**, 4193-4201 (2018)
- [2] Y. Dong, Y. Zou, J. Song, X. Song, H. Zeng, J. Mater. Chem. C **5**, 11369-11394 (2017)
- [3] A. Buffet, A. Rothkirch, R. Döhrmann, V. Körstgens, M. M. A. Kashem, J. Perlich, G. Herzog, M. Schwartzkopf, R. Gehrke, P. Müller-Buschbaum, S. V. Roth, *Journal of Synchrotron radiation* **19**, 647-653 (2012)

Tuning of imprinting stamps for the fabrication of nano-electrodes for electrochemical CO₂ reduction

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Facing global climate change, one of the most important goals is to reduce the concentration of CO₂ in our atmosphere. The photoelectrochemical reduction of CO₂ to climate neutral (solar) fuels is a hot topic in current research. One path to improve the photocatalytic efficiency is to employ large area, nanostructured electrodes. We use lift-off nanoimprint lithography (LO-NIL) to fabricate nano-structured electrodes for CO₂ reduction experiments. In contrast to other nano-lithography techniques, such as electron beam lithography, LO-NIL enables the fast patterning of identical metal nanoisland arrays over large areas [1]. With our

imprinting stamps, we are able to produce arrays with feature sizes of 1400 nm, 350 nm, 200 nm and 75 nm.

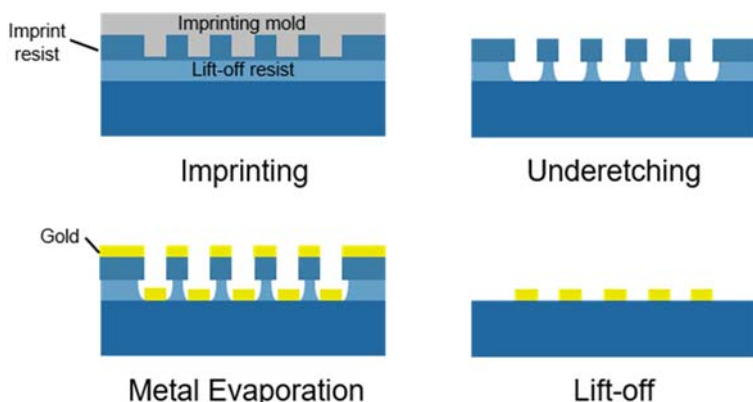


Figure 1: Scheme of the LO-NIL process for metal nano-electrodes.

To further investigate the underlying mechanism, a stepless tuning of the metal nanoislands is required. Using different etching techniques, we are able to reproduce our imprinting stamps in SiO₂. During this reproduction process, the feature size of the stamp can be tuned. The tunability allows analyzing the impact of a changed geometry (such as electrode filling factor, and different aspect ratios of the metal nanoisland circumference and its area) on the electrochemical reactions and their mechanisms. Overall, the geometrical tuning of nano-electrode features provides further understanding of the reaction mechanisms of electrochemical CO₂ reduction.

Electrochemical investigations of these electrodes show that their electrochemical behavior changes drastically with the size of the nanoislands. We observed an increase in catalytic activity with decreasing nanoisland size [2]. Furthermore, the product distribution of the electrochemical CO₂ reduction reaction, catalyzed by the metal nanostructures changes with their size.

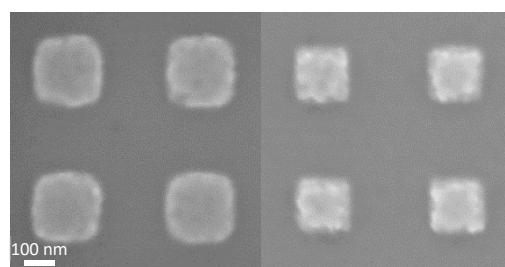


Figure 2: SEM images of an SiO₂ imprinting stamp with (right) and without (left) applied tuning process

References:

- [1] R. D. Nagel *et al.*, "Nanoimprint methods for the fabrication of macroscopic plasmonically active metal nanostructures," *J. Appl. Phys.*, vol. 121, no. 8, p. 084305, Feb. 2017.
- [2] S. Filser *et al.*, "Photoelectrochemical reactivity of well-defined mesoscale gold arrays on SiO₂/Si substrates in CO₂-saturated aqueous electrolyte," *Electrochim. Acta*, vol. 268, pp. 546–553, 2018.

Studying the dynamics of PTB7:PCBM organic photovoltaic active layers

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In organic photovoltaics, electron donor - electron acceptor bulk heterojunctions, as sketched in figure 1 a), are often employed as active material due to their superior performance compared to e.g. planar layered devices. In the optically active polymer, a photon is absorbed and an exciton created. After diffusion to a donor-acceptor interface, the exciton is dissipated and charges can be extracted towards the electrodes and subsequently used, as can be seen figure 1 b).

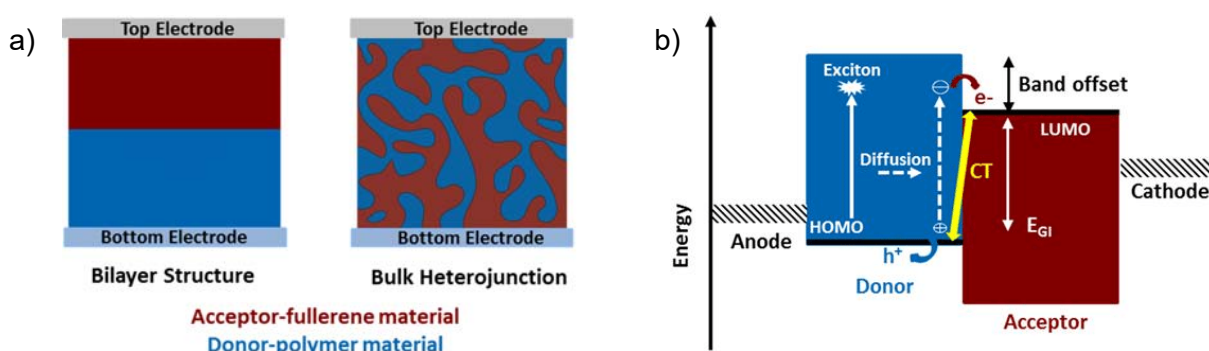


Figure 1: schematic representation of a) two-component active layer structure and b) energy level diagram of such a solar cell [1]

A frequently applied and well-studied system is the combination of P3HT ($(C_{10}H_{14}S)_n$) as electron donor and PCBM ($C_{72}H_{14}O_2$) as electron acceptor. Previous studies have shown, that internal dynamics and structural layout of the active layer influence its electronic properties and thus its performance in a device [2], [3]. A novel, very promising donor material is PTB7 ($(C_{41}H_{53}FO_4S_4)_n$). Structure formulae of the two materials used for this study are depicted in figure 2.

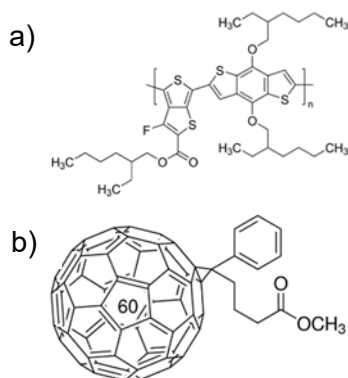


Figure 2: structural formulae of a) PTB7 and b) PCBM

We produced films of PTB7, PCBM and a mixture of these two from a chlorobenzene solution and performed first quasielastic neutron scattering (QENS) experiments on this system in order to evaluate the dynamics of pure compounds as well as blend films on a pico- to nanosecond timescale and potential influences of manufacturing parameters (e.g. mixing ratio, solvent choice, annealing time/temperature ...). QENS experiments were performed in a temperature range between 200K and 400K.

References:

- [1] H. Wang et al. (2014), Materials 7, 2411-2439
- [2] A. Guilbert et al. (2016), The Journal of Physical Chemistry Letters, 7, 2252-2257

Germanium-based nanostructure synthesis guided by amphiphilic diblock copolymer templating

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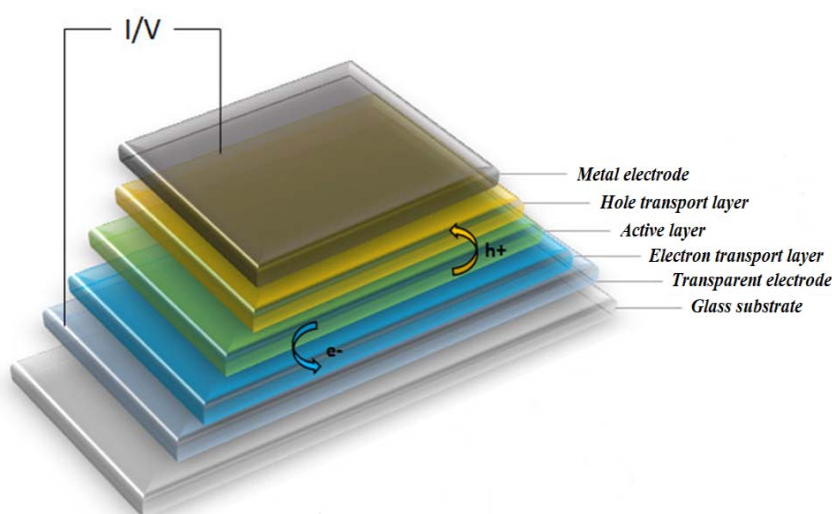
Latest research in the field of hybrid photovoltaics focuses on the benefits of inorganic and organic materials. Flexibility, low cost and large scale production are the most valuable properties of organic components whereas the inorganic components add chemical and physical stability. So far thin films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

Highly Optimized Organic Solar Cells

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Compared to the age of civilization, the Sun presents a timeless source of energy. This fact has, throughout history, inspired many scientists and engineers to find a way to harvest and utilize this power source. With today's increasing energy consumption and demands for ecological standards, usage of renewable energy sources is being strengthened each year [1]. The field of photovoltaics has, consequentially, been in a rapid expansion over the last decade, both in industry and in academics. The ever-growing need for energy is motivating the development of new materials with enhanced photoelectrical properties.



A milestone in the research on organic solar cells has been the invention of bulk-heterojunction solar cells. This allowed for a rapid increase in their efficiency, which has attracted significant attention in recent years. Modern tandem photovoltaic devices with polymer-based active layer reach the power conversion efficiency of up to 17.3% [2]. Properties such as light weight, flexibility, band-gap tunability and semitransparency, allow a wide range of application in the field of electronic devices. In addition, contemporary polymer materials have enabled several solution-based processing techniques, making low-cost fabrication of organic solar cells at large scale possible.

Organic solar cells can be fabricated both in standard or inverted architecture. The two architectures differ in the placement of the electron and the hole transport layer – their position is inverted. We have primarily focused on the inverted architecture (shown in the figure) since it has been demonstrated to be more stable [3], mainly due to better matching of the energy levels and chemical compatibility of the active layer materials with materials most commonly used as blocking layers. The power conversion efficiency highly depends on the thickness and morphology of the active layer and the charge carrier transport layers. Layer thicknesses and annealing methods that yielded the highest power conversion efficiencies have been determined. Further optimization of the solar cells was carried out by insertion of interlayers between the active layer and the respective electrode, and by patterning the photoactive area of the cell. Following these processing techniques, achieved fill factors are close to the theoretical maximum set for solar cells [4].

References

- [1] V. Smil, *Energy Transitions: Global and National Perspectives*, Prager (2016) 2nd Edition, USA.
- [2] L. Meng et al, *Science* 361, 1094-1098 (2018).
- [3] D. Han, S. Yoo, *Sol. Energy Mater Sol. Cells* 128, 41-47 (2014).
- [4] W. Shockley, H. J. Queisser, *J. Appl. Phys.* 32, 510-519 (1961).

Analysis of Redox-Flow Batteries for centralised storage applications in low-voltage grids

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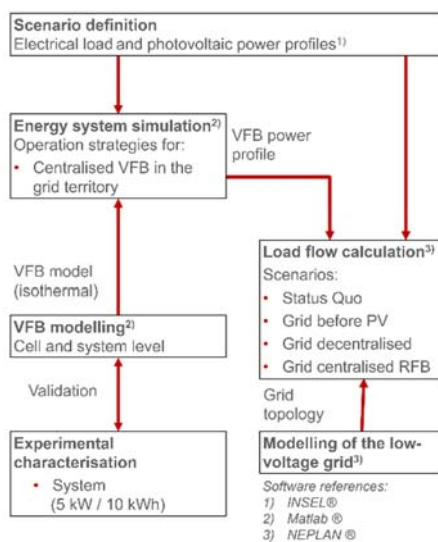


Figure 1: Simulation concept

The use of electrical energy storages most likely increases the electrical self-sufficiency of a grid segment and offers a high potential for compensation of grid stability problems. The following research approach concerns the possible potentials of Vanadium Redox-Flow Batteries (VRFB) for the long-term use in large central storage systems. The high reusability of the electrolyte due to possible retreatment allows a sustainable use as energy storage system. Compared to smaller VRFB in decentralised applications central storages offer economic scale-up effects of components and maintenance. Moreover, the investment costs of the presented approach are bundled, so that the total cost of ownership is decreased. The abstract presents the systematic concept for a system simulation of VRFB for centralised storage applications in low-voltage grids.

In order to examine the aforementioned context, the concept shown in figure 1 is developed. Based on the scenario definition, the electrical load and the photovoltaic power profiles are derived. These profiles are used as input for the energy system simulation and the load flow calculation, described below. The experimental characterization of a

VRFB system (5 kW / 10 kWh) provide the data set for the mathematical VRFB modelling. Based on the model published in [1], a simplified isothermal VRFB model for the use in the energy system simulation is developed. Within this simulation, operation strategies for the local energy balancing based on the economical concept of the VRFB are defined. The output of the simulation is the actual VRFB power profile, which is the second input of the load flow calculation. The load flow calculation is based on a model of a typical low-voltage grid topology [2] and shows the utilization of grid components and the power quality. Due to the comparison of the historical grid usage before and after the photovoltaic integration and a grid with photovoltaics combined with a centralised VRFB system (figure 2), the performance of the low-voltage grid in each scenario can be evaluated.

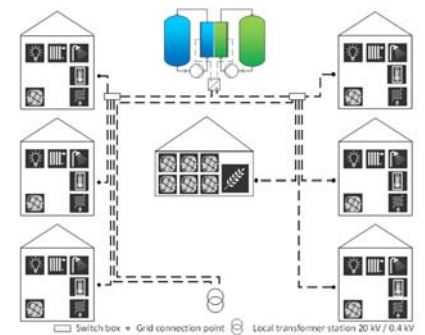


Figure 2: Centralised VRFB

Future impacts of the work presented can be an improved and validated commercialization concept for centralised Redox-Flow Batteries (figure 2). Therefore, adapted local marketing strategies for decentralised power generation units are defined and evaluated. Finally, the avoidance of additional local grid extension measures due to the use of centralised VRFB systems can be analysed. The evaluation of energy systems in low-voltage grids in combination with the commercialization concept shows a holistic approach for the prospective use of Redox-Flow Batteries.

References:

- [1] König, Sebastian (2017): Model-based Design and Optimization of Vanadium Redox Flow Batteries. Dissertation. Karlsruher Institut für Technologie (KIT), Karlsruhe. Fakultät für Elektrotechnik und Informatik.
- [2] G. Kerber, Aufnahmefähigkeit von Niederspannungsverteilnetzen für die Einspeisung aus Photovoltaikkleinanlagen, Dissertation, Technische Hochschule München, 2011.

Highly-Regular Porous Antimony Oxide Thin Film Electrode for Rechargeable Batteries

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Due to limited supply of traditional fossil fuels, increasing carbon emission, and deteriorated environmental pollution, it is urgent for humankind to ensure alternative renewable energy sources.

Due to high energy density, competitive working voltage, minimum self-discharge, and limited maintenance requirements, rechargeable lithium-ion batteries (LIBs) have been applied in various fields and regarded as the most promising power devices in the future. In recent years, the shortage of lithium source gradually became a noteworthy problem, which could limit the development of LIBs in next years. Since that sodium is an earth abundant material and sodium-ion batteries (SIBs) can meet these requirements better than LIBs, SIBs have come up as a more suitable alternative to LIBs for these applications[1]. Due to high theoretical capacity (Sb_2O_4 for 1220 mAh g^{-1} , Sb_2O_3 for 1102 mAh g^{-1}), appropriate reaction potential and abundant reserves in the earth crust, antimony oxides are regarded as a promising alternative anode materials which could be applied in both LIBs and SIBs[2]. However, antimony oxides suffer from volume expansion during charge and discharge, leading to a rapid capacity fading. Creating hollow or porous structure is an effective strategy to improve cycling stability of antimony oxides anodes, because it can provide enough void space to accommodate volume changes of antimony oxides[3].

Herein, we propose a novel method to synthesize highly-regular porous antimony oxide tin film anode materials assisted with block copolymer. Amphiphilic block copolymers (ABC) have been widely utilized as surface modification agents by constructing nanoscale architectures on various substrates through evaporation induced self-assembly processes[4]. Polymer/inorganic nanocomposites can be obtained via a microphase separation process in mixture solution of mixing block copolymer and precursor of metal oxide. Moreover, the morphology of nanocomposites could be controlled accurately by altering synthesis conditions[5]. After calcination, nanostructured metal oxide materials are gained. The morphology of as-prepared porous antimony oxide tin film anodes could be characterized by scanning electron microscopy (SEM) partially and grazing incidence small angle X-ray scattering (GISAXS) integrally[6]. Furthermore, in operando SAXS or Small-angle neutron scattering (SANS) measurements can be applied to investigated the evolving nanoscale morphology of electrode during charge and discharge processes[7, 8].

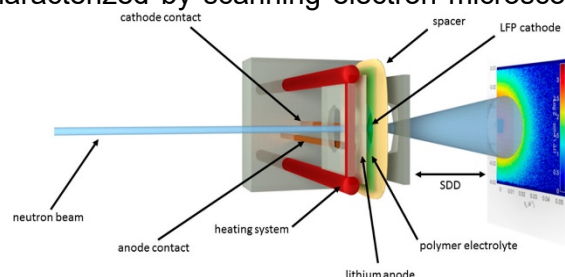


Figure 2: Schematic of the full battery operando SANS setup with the battery components, contacts, and heating unit. Ref. [8]

References

- [1] S.P. Ong, V.L. Chevrier, G. Hautier, A. Jain, C. Moore, S. Kim, X. Ma, G. Ceder, *Energy & Environmental Science*, 4 (2011) 3680-3688.
- [2] N. Li, S. Liao, Y. Sun, H.W. Song, C.X. Wang, *Journal of Materials Chemistry A*, 3 (2015) 5820-5828.
- [3] J. Pan, N. Wang, Y. Zhou, X. Yang, W. Zhou, Y. Qian, J. Yang, *Nano Research*, 10 (2017) 1794-1803.
- [4] Y. Deng, J. Wei, Z. Sun, D. Zhao, *Chemical Society Reviews*, 42 (2013) 4054-4070.
- [5] Y.J. Cheng, J.S. Gutmann, *Journal of the American Chemical Society*, 128 (2006) 4658-4674.
- [6] P. Müller-Buschbaum, *Advanced Materials*, 26 (2014) 7692-7709.
- [7] G.E. Mohl, E. Metwalli, P. Muller-Buschbaum, *Acs Energy Letters*, 3 (2018) 1525-1530.
- [8] G.E. Möhl, E. Metwalli, R. Bouchet, T.N.T. Phan, R. Cubitt, P. Müller-Buschbaum, *ACS Energy Letters*, 3 (2017) 1-6.

Interfaces in polymer based thin-film lithium-ion batteries

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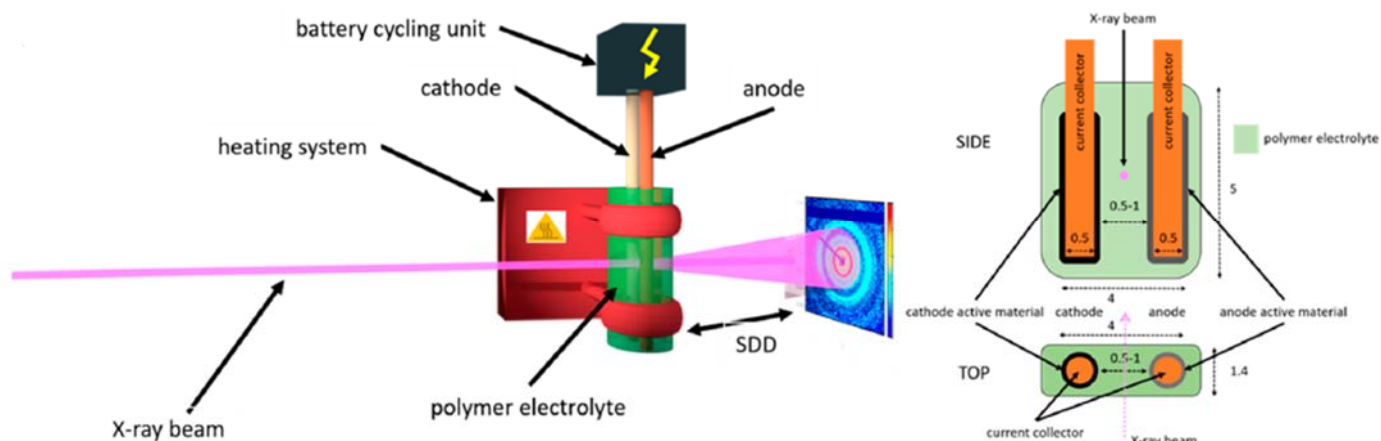


Figure 1: Sketch of the in-operando small-angle X-ray scattering (SAXS) measurement setup on solid state polymer lithium-ion batteries. The left part shows an overview of the setup while the right part visualizes the measured capillary battery. Dimensions are given in millimeters. [1]

With rising importance and amount of non-constant renewable energy sources the need for reliable and highly efficient energy storage-solutions grows. Since batteries are not only to be used in stationary but also in electric vehicles and mobile electronic devices, further research is needed to increase efficiency, reliability and life time while reducing weight, volume and production costs. Most batteries used currently in the industry are lithium ion batteries (LIBs) with liquid electrolytes based on technologies commercialized in 1991. LIBs combine high energy and power capacity compared to other battery technologies. Due to the inflammable nature of liquid electrolytes LIBs are prone to dangerous damage upon mechanically or temperature induced leakage. Solid state batteries based on polymers can overcome these issues due to their mechanical and temperature stability. However the ionic conductivity which is related to the morphology of the electrolyte, still needs to be increased. Polyethylene oxide (PEO) is a well known Li-ion conducting polymer. Its shortcomings in terms of physical stability can be compensated by using block copolymer electrolytes (BCEs). Combining the different advantages of the the polymer blocks and their nanoscale structures, they offer many possibilities for optimization. Changing the block length or the solvent environment in the process can be used to manipulate the morphology of the BCE system. Polystyrene-*block*-polyethylene oxide (PS-*b*-PEO) has been investigated extensively as electrolyte. The PS block offers mechanical stability while the PEO part ensures ionic conductivity. Adding the lithium salt lithium bistrifluoromethanesulfonimide (LiTFSI) provides the necessary lithium-ions as charge carriers for the electrolyte. Capillary batteries are built using this polymer electrolyte. In-operando SAXS measurements, as seen in figure 1, provide insight into changes in the polymer's morphology, in bulk as well as at the interfaces of electrolyte and electrodes during charge and discharge. The contrast between the blocks, caused by different electron densities, allows for an analysis of the electrolyte's structural evolution in nanometer scale by nondestructive scattering experiments. Previous works have already shown the importance of in-operando measurements which create essential realistic conditions and yield to new insights in the needs for a successful design of polymers in LIBs. [1]

References

- [1] G. Möhl, E. Metwalli, In Operando Small-Angle X-ray Scattering Investigation of Nanostructured Polymer Electrolyte for Lithium-Ion Batteries, ACS Energy Lett. 2018, 3, 7, 1525-1530

Revealing the growth of copper as contacts for polymer thin film lithium-ion batteries

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Understanding the interface between metals, commonly used as current collectors, and ion-conducting polymers used in polymer lithium-ion batteries (LIBs) is crucial to develop highly reproducible, low-cost and reliable devices. To address these issues, sputter deposition is the technique of choice to fabricate scalable, reproducible and controllable nanometer and sub-nanometer metal layers on polymer thin films. The sputter deposition process, being well understood and controlled, offers advantages over chemical methods to tailor metal thin-film morphologies on the nanoscale and offers a superior adhesion of the deposited material.[1] We use in-situ grazing incidence small angle X-ray scattering (GISAXS) to investigate the formation, growth and, self-assembled structuring on polymer thin films used in LIBs.[2]

The growth of gold on silicon and homopolymer substrates was investigated by Schwartzkopf et al. [1],[2]. Continuing these studies having a polymer solid-state LIB in mind, the growth of copper on polystyrene-*block*-poly(ethylene oxide) (PS-*b*-PEO), a diblock copolymer with a glassy PS block providing mechanical stability and a soft, ion-conducting PEO block, used for polymer electrolytes and composite battery electrodes is investigated. As the sputter deposition of copper is, as for gold, a cluster-like growth and not a layer by layer growth, it can be described using a slightly modified hemispherical growth model by Schwartzkopf et al. [3]. Also a selective growth of copper on the different polymer domains is found in the GISAXS measurements. Thus, this work gives valuable insight into understanding the growth mechanism of copper current collectors on polymer composite electrodes for LIBs.

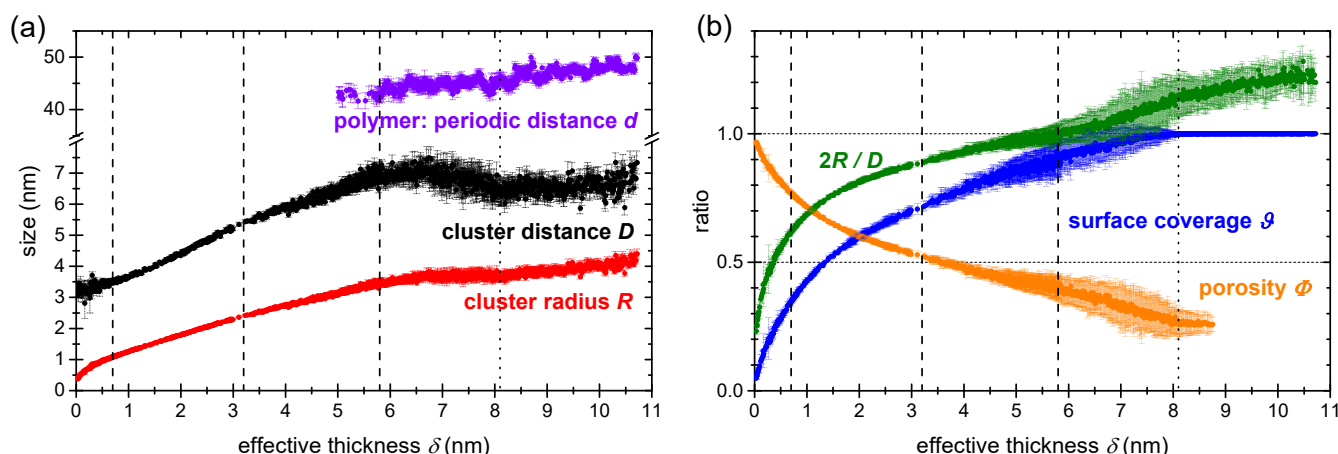


Figure 1: (a) evolution of extracted polymer domain distance d , metal cluster distance D , and radius R with effective metal layer thickness δ ; (b) calculated ratio $2R/D$, surface coverage θ , and porosity ϕ against the effective metal layer thickness δ .

- [1] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017).
- [2] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).
- [3] Schwartzkopf et al., Nanoscale 5, 5053 (2013).

Structural and electrochemical properties of “disordered, spinel-like” structures derived from NCM materials by chemical delithiation

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Future Li-ion batteries are required to have higher energy densities, which most likely can be achieved by improving the specific capacity of cathode active materials (CAMs). The most promising and commercially used cathode active material is the layered $\text{LiNi}_x\text{Co}_y\text{Mn}_z\text{O}_2$ (NCM, with $x+y+z=1$) due to its high achievable specific capacity, high power and energy densities, its good structural stability and a small volume change during cycling.^[1] The present work is aimed at the charging (delithiation) process of NCM since deleterious O_2 evolution is observed from the NCM surface lattice at high degrees of delithiation (~80% SOC).^[1] This is accompanied by the formation of a disordered spinel (M_3O_4) and/or rock salt (MO) phase on the NCM particle surface.^[2,3]

Oxygen release from partially delithiated NCM can also be achieved thermally, while an increasing Ni content aids in thermal oxygen release by lowering the onset temperature and increasing the released oxygen amount.^[3,4] Thermogravimetric Analysis coupled with Mass Spectrometry (TGA-MS) results of electrochemically delithiated electrodes (80% SOC) showed a simultaneous CO_2 and O_2 evolution similar to the electrochemically induced oxygen release.^[2] However, these experiments face the problem of impurities from the binder, conductive carbon or electrolyte on the electrochemically delithiated electrodes, which is why heating of e.g. chemically delithiated NCM material (until the destabilization of the structure) could produce quantitative and cleaner O_2 release data directly from the CAM.

The detailed study of such chemically delithiated NCM materials using electrochemical testing methods, TGA-MS, X-ray Diffraction (XRD) and X-ray Photoelectron Spectroscopy (XPS) is the main objective in this work. By electrochemical cycling, we confirmed the chemical delithiation of the observed NCM material using the oxidation agent NO_2BF_4 in acetonitrile medium. TGA-MS was used to determine the oxygen release behavior of the chemically delithiated samples and XRD analysis lead to the observation of a spinel phase after thermal oxygen depletion. XPS further confirmed a structural surface phase transition of the chemically delithiated material. The obtained results help for a better understanding of the processes happening during the oxygen release of NCM materials.

[1] R. Jung, M. Metzger, F. Maglia, C. Stinner, H. A. Gasteiger, J. Electrochem. Soc. 2017, 164, A1361–A1377.

[2] J. Wandt, A. T. S. Freiberg, A. Ogrodnik, H. A. Gasteiger, Mater. Today 2018, 21, 825–833.

[3] H. J. Noh, S. Youn, C. S. Yoon, Y. K. Sun, J. Power Sources 2013, 233, 121–130.

[4] S.-M. Bak, E. Hu, Y. Zhou, X. Yu, S. D. Senanayake, S.-J. Cho, K.-B. Kim, K. Y. Chung, X.-Q. Yang, K.-W. Nam, ACS Appl. Mater. Interfaces 2014, 6, 22594–22601.

Delving into Lithium-Ion Battery Anode Material Graphite: Investigation of Rate Limiting Parameters by Overpotential Deconvolution

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Fast charging of lithium-ion batteries requires an electrode design, that minimizes the total overpotential. In a porous graphite electrode, there are three major domains that cause overpotentials: The solid phase, the liquid phase inside of the pores and the interface in between of these two domains. During charging, first, the lithium ions pass through the liquid phase, where the transport is restricted by the resistivity of the electrolyte and diffusion (c.f. Figure). Then, at the particles surface, the ions pass through the solid electrolyte interface (SEI) and lithium intercalates into the solid phase. Inside the particles, a concentration gradient from surface to centre induces lithium diffusion, which comes again with an overpotential. Depending on each particles size, shape and position in the electrode, the domains contribute differently to the total overpotential. It is difficult to deconvolute the contributions, so that an improved experiment design is necessary.

We will investigate graphite electrodes and deconvolute the total overpotential by different electrode designs. Thus, for the electrode preparation, sieved graphite powders are used to ensure a well-defined characteristic length of the system. Reducing the thickness of the electrode will vanish the contribution of the liquid phase to the total overpotential. Secondary, we will perform electrochemical impedance spectroscopy (EIS) to differentiate between the different resistances at different frequencies.

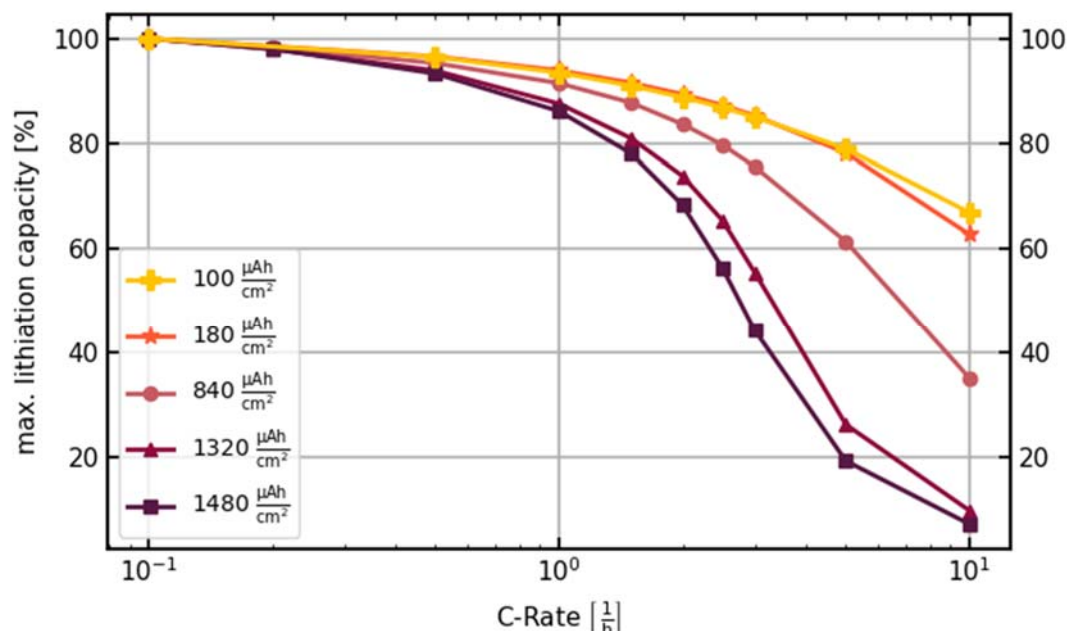


Figure 1: Rate test of graphite electrodes with varied thickness

At elevated C-rates the attainable capacities are smaller for larger thicknesses (higher loading). This indicates a limitation due to the liquid phase.

Analysis of metal nanostructure evolution on polymer surfaces by in-situ GISAXS during sputter deposition

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A good understanding of the fabrication process of reproducible functional metal-polymer interfaces is of high importance for their use in organic electronics. Sputter deposition offers the ability to precisely control and tailor the fabrication of metal-polymer interfaces. During sputter deposition, the evolution of the metallic layer morphology is monitored in situ with time-resolved grazing-incidence small-angle X-ray scattering (GISAXS). The resulting in-situ scattering data is processed and analyzed using the DPDAK software package [1]. By fitting the processed data, structure parameters can be extracted which temporal evolution reveals the mode of metal growth on polymer surfaces.

For each sample, vertical line cuts are performed at $q_y = 0$, which are fitted with Gaussian functions. The measured distance Δq_z between two adjacent peaks allows the determination of an average film thickness δ using the simple relation $\delta = \frac{2\pi}{\Delta q_z}$. For each sample, two narrow horizontal cuts are performed at the Yoneda positions of the corresponding metal and polymer as well as one broad Yoneda cut. As peaks are arising in the horizontal cuts, it is evident that the metal growth happens not layer by layer but as a growth of single metal clusters on the polymer surface until a complete metal layer is formed. The horizontal cuts are fitted with a combination of Lorentzian and Gaussian functions, which allows tracking of the position of the side peaks and, consequently, the determination of the temporal evolution of the cluster distance $D = \frac{2\pi}{q_y}$. The cluster radius R is computed by employing a simplified geometrical model [2-4].

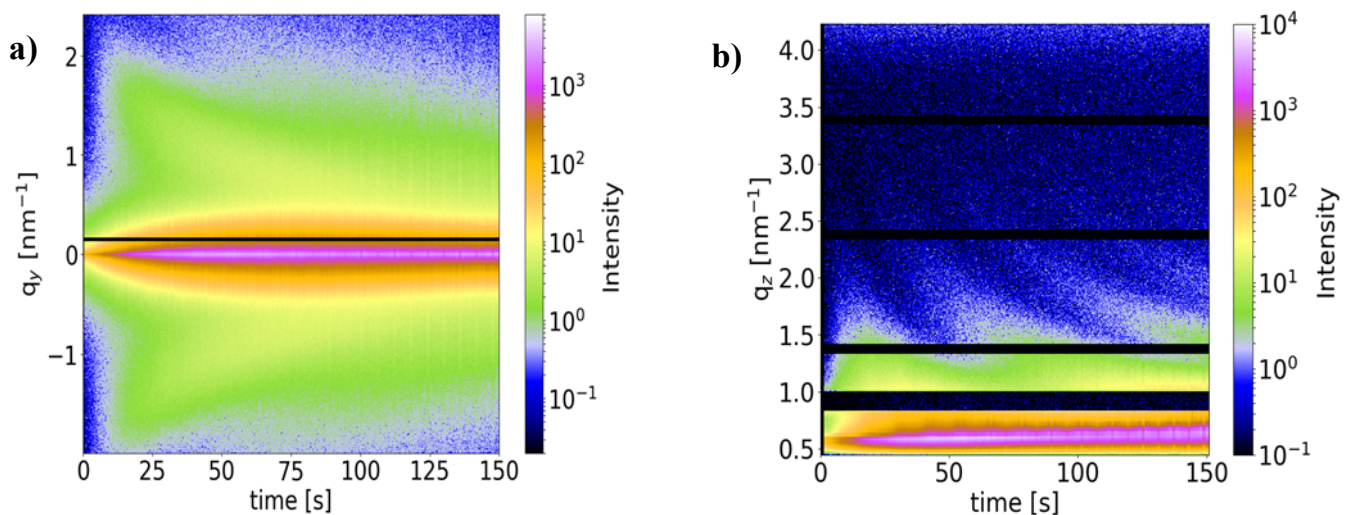


Figure 1: (a) 2D map showing the temporal intensity evolution of horizontal cuts. (b) 2D map showing the temporal intensity evolution of vertical cuts.

- [1] Benecke et al., J. Appl. Cryst. 47, 1797-1803, (2014)
- [2] Schwartzkopf et al., Nanoscale 5, 5053 (2013).
- [3] Schwartzkopf et al., ACS Appl. Mater. Interfaces 7, 13547 (2015).
- [4] Schwartzkopf et al., ACS Appl. Mater. Interfaces 9, 5629 (2017).

Space-Charges in Solid Electrolytes: negligible impact?

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The search for materials and technologies for the next generation of electric vehicles is versatile. All-Solid-State Batteries (ASSB) could enable Li-metal anodes and the use of non-flammable materials. The energy density and safety could improve greatly once the challenges currently faced are overcome. The major bottleneck in ASSB is posed by the interfaces between the different materials, solid anode/electrolyte/cathode.

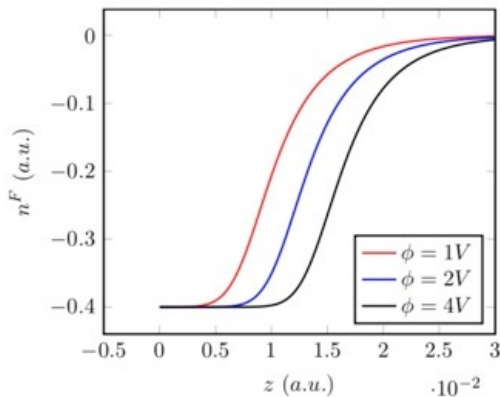


Figure 1: Charge(Li⁺) distribution near anode/electrolyte interface

Therefore, the main performance limitation has been assigned to the properties of the electrode/electrolyte interface. A fundamental phenomenon, when two different materials are brought into contact, the accumulation and depletion of charges, has been only sparsely covered by experimental and theoretical work for solid electrolytes.

Different theoretical models suggest thicknesses of the depletion layers between several nanometers and several micrometers, whereas experiments have the same discrepancies.

To-date, there are no literature reports proving the existence and scale of the space-charge-layers. In this work, we perform theoretical and experimental studies on a LISICON electrolyte and propose a model, which is capable to explain the impedance response of this electrolyte within the framework of existing interfacial depletion layers.

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Solid Solutions of Lithium Phosphidotetrelates – Tailoring Solid-State Ion Conductors

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Solid electrolytes with high ionic conductivity and chemical stability are the key component for full-scale commercialization of all-solid-state batteries. The mobility of lithium ions in solid electrolytes depends on the diffusion pathway, which can be modified by substituting differently sized ions into the structure.^[1-2] Recently, we investigated several lithium phosphidosilicates and -germanates, which proved to be good lithium ion conductors with conductivities up to $1.2 \cdot 10^{-4} \text{ S cm}^{-1}$ at 75°C . Compared to sulfide and oxide based lithium ion conductors, phosphide based materials exhibit an increased lithium content and, therefore a higher charge carrier concentration, due to the higher negative charge of the phosphide anion.^[3-4]

We present a solid solution of the lithium conductors Li_8SiP_4 ($4.5 \cdot 10^{-5} \text{ S cm}^{-1}$)^[3,4] and $\alpha\text{-Li}_8\text{GeP}_4$ ($1.8 \cdot 10^{-5} \text{ S cm}^{-1}$)^[4] with the nominal composition $\text{Li}_8\text{Ge}_x\text{Si}_{1-x}\text{P}_4$, which crystallizes in the cubic space group $P\bar{a}3$ (205). Figure 1 shows the crystal structure. The Vegard plot in figure 2 describes the linear dependence of the cell parameter a on the substitution grade x in $\text{Li}_8\text{Ge}_x\text{Si}_{1-x}\text{P}_4$ with $x=0/0.25/0.5/0.75/1$. The solid solution is yielded via a mechanochemical synthesis with subsequent annealing as crystallographic pure phase over the entire investigated range.

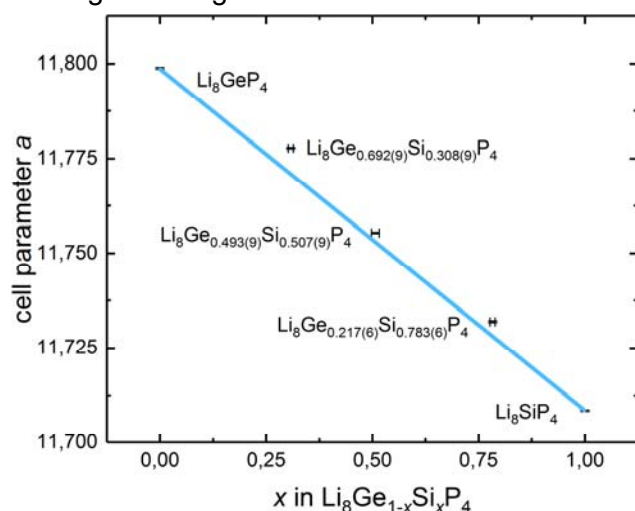


Figure 2: Vegard plot of $\text{Li}_8\text{Ge}_x\text{Si}_{1-x}\text{P}_4$. The Si content x is refined by the Rietveld method from powder X-ray diffraction measurements.

References

- [1] J. Janek, W. G. Zeier, *Nat. Energy* **2016**, 1, 16141.
- [2] J. C. Bachman, S. Muy, A. Grimaud, H.-H. Chang, N. Pour, S. F. Lux, O. Paschos, F. Maglia, S. Lupart, P. Lamp, L. Giordano, Y. Shao-Horn, *Chemical Reviews* **2016**, 116, 140-162.
- [3] L. Toffoletti, H. Kirchhain, J. Landesfeind, W. Klein, L. van Wüllen, H. A. Gasteiger, T. F. Fässler, *Chem. - Eur. J.* **2016**, 22, 17635-17645.
- [4] Eickhoff, H.; Strangmüller, S.; Klein, W.; Kirchhain, H.; Dietrich, C.; Zeier, W. G.; van Wüllen, L.; Fässler, T. F. *Chem.-Mater.* **2018**, 30, 6440-6448.

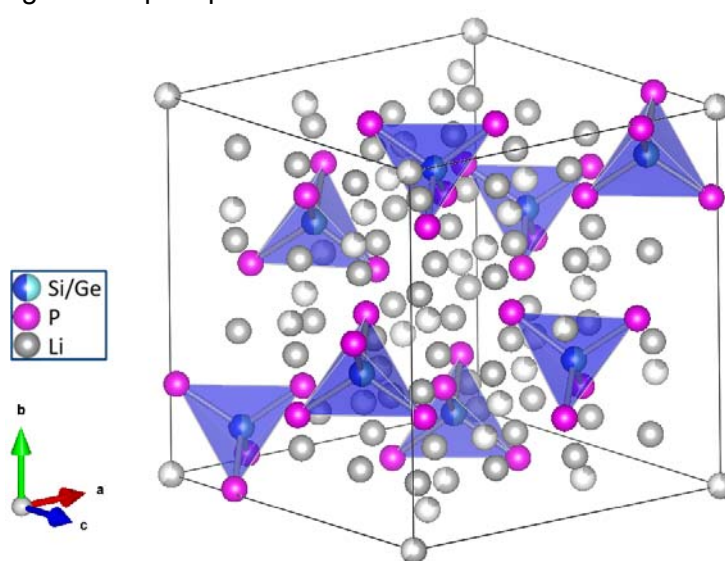


Figure 1: Crystal structure of Li_8SiP_4 and $\alpha\text{-Li}_8\text{GeP}_4$. The phosphorus atoms form a fcc lattice, where the silicon and germanium atoms occupy 1/8 of the tetrahedral voids. Lithium fills the remaining tetrahedral voids as well as parts of the octahedral voids.

We investigated the effect of the lattice parameter a on the ionic conductivity via impedance spectroscopy, using a cell setup with elevated pressure, so the samples are pelletized in situ. By measuring at different temperatures we can extract the activation energy from an Arrhenius plot. We also show the solid solution $\text{Li}_8\text{Ge}_x\text{Si}_{1-x}\text{P}_4$, which crystallizes in space group $P\bar{4}3n$ (218) same as $\beta\text{-Li}_8\text{GeP}_4$.

Li₁₄SiP₆ – A Fast Lithium Ion Conductor

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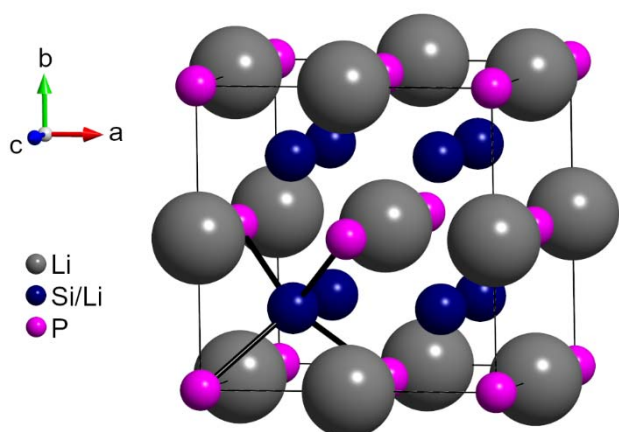


Figure 1: Structure of Li₁₄SiP₆ at 4 K. Li, Li/Si (mixed site) and P atoms are depicted as grey, indigo and pink thermal ellipsoids, respectively, set at 90% probability. Thick black lines mark (Li/Si)-P bonds resulting in a (Li/Si)P₄ tetrahedron.

Herein, the preparation and characterization of the new lithium-rich phosphidosilicate Li₁₄SiP₆ is reported. In order to increase the charge carrier density of lithium phosphidosilicates, Li₁₄SiP₆ was synthesized applying a two-step synthesis route combining mechanochemical ball milling and subsequent annealing of the obtained reactive mixture. Characterization via X-ray diffraction (powder and single crystal) and elastic coherent neutron scattering experiments enabled the thorough investigation of the structural and thermal behavior of the compound (Figure 1). Activation energies, ionic and electronic conductivities have been determined using solid state ⁷Li NMR measurements as well as electrochemical impedance spectroscopy. Finally, diffusion pathways were analyzed by temperature dependent powder neutron diffraction measurements in combination with MEM and DFT calculations to extend the knowledge about the material properties (Figure 2).

References:

- [1] Z. Zhang, Y. Shao, B. Lotsch, Y. Hu, H. Li, J. Janek, L. F. Nazar, C. Nan, J. Maier, M. Armand and L. Chen, *Energy Environ. Sci.* **2018**.
- [2] L. Toffoletti, H. Kirchhain, J. Landesfeind, W. Klein, L. v. Wüllen, H. A. Gasteiger and T. F. Fässler, *Chem. Eur. J.* **2016**, *22*, 17635.
- [3] H. Eickhoff, L. Toffoletti, W. Klein, G. Raudaschl-Sieber and T. F. Fässler, *Inorg. Chem.* **2017**, *56*, 6688.
- [4] A. Haffner, T. Bräuniger and D. Johrendt, *Angew. Chem. Int. Ed.* **2016**, *55*, 13585.
- [5] H. Eickhoff, S. Strangmüller, W. Klein, H. Kirchhain, C. Dietrich, W. G. Zeier, L. v. Wüllen and T. F. Fässler, *Chem. Mater.* **2018**, *30*, 6440-6448.

Recently, the development of all-solid-state batteries as high power and energy density storage devices has become one of the key challenges in solid state chemistry and material science. Not only improvement of current electrode and electrolyte materials as well as the cell architecture, but also the search for new compounds is necessary to get access to a new generation of all-solid state battery technology.[1]

Recently, a new class of promising lithium ion conductors has been studied intensively. Lithium phosphidosilicates and -germanates offer, analogously to oxidosilicates, thiosilicates and thiophosphates, a large structural variety combined with decent lithium ion conductivity up to 10⁻⁴ S cm⁻¹ at 25 °C.[2-5]

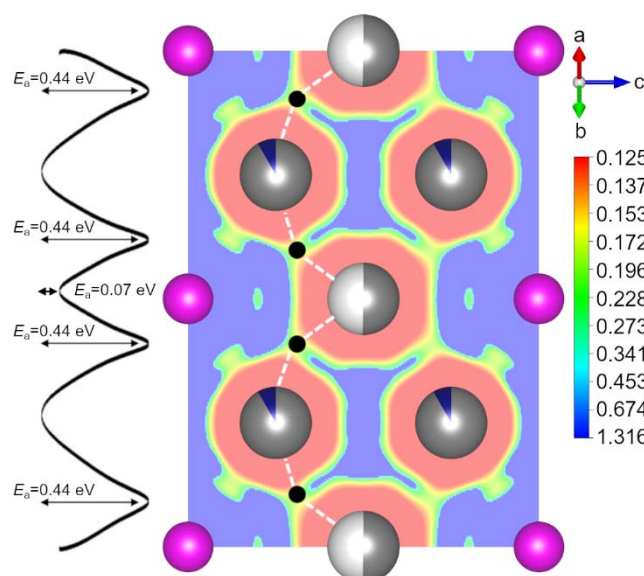


Figure 2: 2D section cut (110, d = 1 plane) of the lithium one-particle-potential (OPP) and its 1D section along lines connecting five Li atoms in a chain Li2-•-Li1-•-Li2-•-Li1-•-Li2, where • corresponds to the neck connecting neighboring sites with partial Li occupations.

Diffraction studies of prismatic Li-ion batteries with neutrons and high energy X-ray diffraction

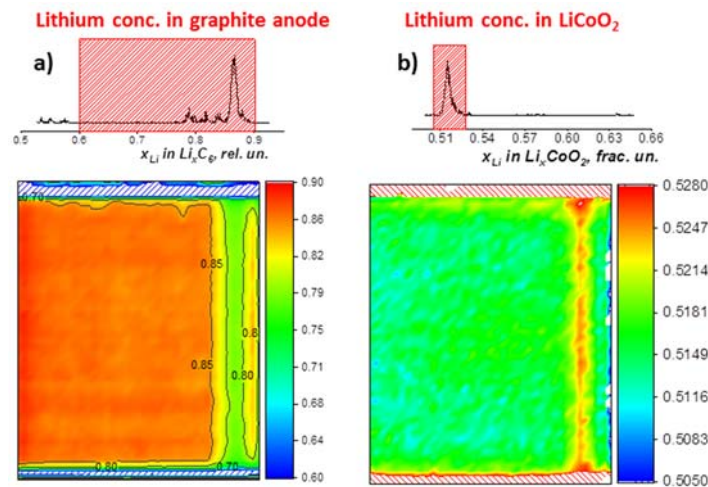
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Currently, Li-ion batteries occupied an important role in energy market and are widely used in powering portable devices, off-grid energy storage, and e-mobility applications. Despite characteristics of modern Li-ion batteries (LIBs) (high power/energy density, high mass and volumetric capacities, nearly no memory effect, low self-discharge when not in use etc.) there is still a certain room for improvement of selected characteristics, e.g. cell capacity, safety, cycle life, temperature stability, cost etc. This makes research on LIBs of high scientific and technological relevance [1].

Of particular interest are methods which allow performing *in situ* / *operando* studies. Powder diffraction is a well-established experimental method well suited for studies of LIBs on atomic scale [2]. Among different diffraction sources - lab X-rays, synchrotron radiation and thermal neutrons – last two are of great value since they are capable to probe the structure of Li-ion cell components under real operating conditions without dismantling the cell, and can be also used for non-ambient operating conditions.

Recently we showed by means of high energy X-ray diffraction 2D Li distribution in the anode and the cathode of the commercial prismatic Li-ion cell (Figure 1) [3]. For the same prismatic battery by means of neutron diffraction, we find out the overall Li concentration in the cell from results of Rietveld refinement (Figure 2a,b) and more importantly we were able to observe phases evolution inside the cell for *operando* conditions (Figure 2c,d) [4]. In the current contribution, we would like to present capabilities of these two methods in the studies of prismatic Li-ion



batteries, in particular for *in situ* / *operando* conditions.

Figure 1: 2D distribution of Li concentration in the anode (a) and the cathode (b) of the prismatic Li-ion battery.

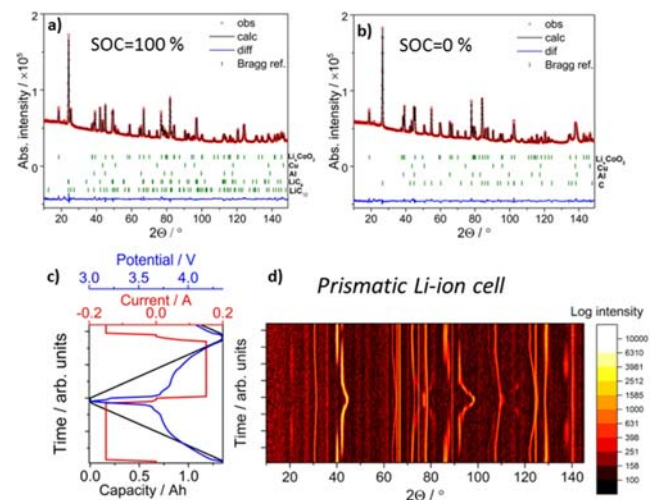


Figure 2: Rietveld refinement of neutron powder data for prismatic battery in SOC=100 % (a) and SOC=0 % (b). Evolution of electrochemical parameters (c) and stack of neutron diffraction patterns (d) (background subtracted log diffraction intensity coded in false color vs. 2θ) collected for prismatic Li-ion battery.

- [1] 1. Ehrenberg, H., et al., In Situ Diffraction Measurements: Challenges, Instrumentation, and Examples., in Modern Diffraction Methods (528), I.E.J.M.U. Welzel, Editor. **2012**, Wiley-VCH: Weinheim.
- [2] Harks, P.P.R.M.L., F.M. Mulder, and P.H.L. Notten, In situ methods for Li-ion battery research: A review of recent developments. J. Power Sources, **2015**, 288, 92-105.
- [3] M. J. Mühlbauer, A. Schökel, M. Etter, V. Baran, and A. Senyshyn, J. Power Sources, **2018**, 403, 49-55.
- [4] V. Baran, M. Mühlbauer, M. Schulz, J. Pfanztelt, and A. Senyshyn, J. Storage Mater., submitted.

Intermetallic Tetrel Element compounds as Wet Chemical Precursors for Porous, Thin Films

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Hybrid solar cells combine the unique properties of inorganic semiconductors and organic polymers which result in low production costs and flexibility.^[1] However, routes to periodic porous materials are scarce. Oxidative decomposition of ZINTL clusters in presence of a specific template leads to homogenous thin films. So far, we succeeded in preparing germanium films with inverse opal morphology and a well-defined pore size in the range of 300 nm using solutions of the intermetallic compound K_4Ge_9 which contains nine-atomic clusters.^[2] Also, we succeeded in showing the use of these materials as an anode material in Li-ion batteries.^[3] Moreover we were able to prepare nanoporous films using an amphiphilic diblock copolymer as a structure controlling template.^[4]

Herein we present a wide variety of intermetallic compounds that can be utilized in this wet chemical approach as well. Mixed Si-Ge and Sn-Ge compounds as well as Si and Sn compounds lead to inverse opal structured thin films while Sn-Bi compounds lead to a macroporous thin film structure. On top of that, we highlight carrier dynamics in some of these materials using Time Resolved Terahertz Spectroscopy (TRTS).

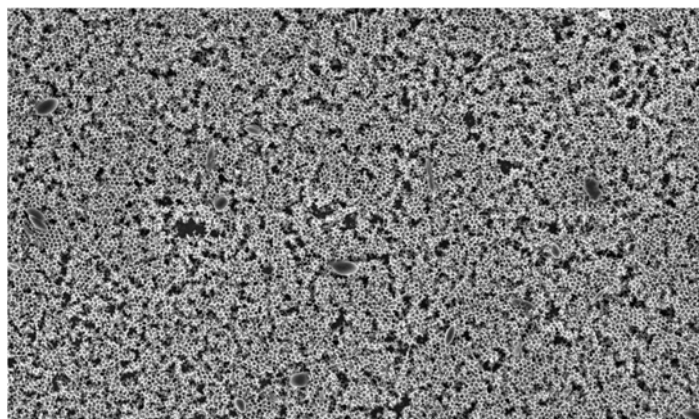


Figure 1: SEM of a Ge_xSi_{1-x} -film ($x = 0.75$) showing inverse opal structured material throughout a large area

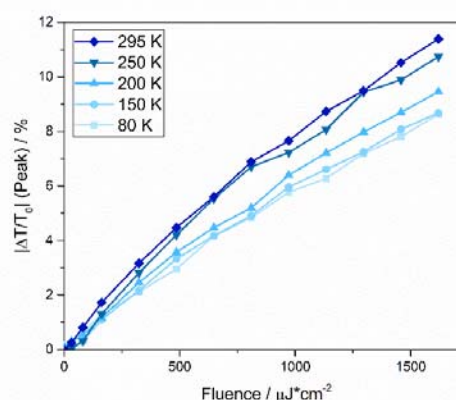


Figure 2: TRTS of a Ge_xSi_{1-x} -film ($x = 0.75$). Temperature as well as fluence dependency of peak signal. ΔT : change in transmittance

- [1] S. Günes, N. S. Sariciftci, Inorg. Chim. Acta 2008, 361, 581-588.
- [2] M. M. Bentlohn, M. Waibel, P. Zeller, K. Sarkar, P. Müller-Buschbaum, D. Fattakhova-Rohlfing, T. F. Fässler, Angew. Chem. Int. Ed. 2016, 55, 2441-2445. DOI: 10.1002/anie.201508246.
- [3] S. Geier, R. Jung, K. Peters, H. A. Gasteiger, D. Fattakhova-Rohlfing, T. F. Fässler, Sustainable Energy Fuels 2018, 2, 85-90.
- [4] N. Hohn, A. E. Hetzenecker, M. A. Giebel, S. Geier, L. Bießmann, V. Körstgens, N. Saxena, J. Schlipf, W. Ohm, P. S. Deimel, F. Allegretti, J. V. Barth, S. V. Roth, T. F. Fässler, P. Müller-Buschbaum, Nanoscale 2019, 11, 2048-2055.

A Design Approach for Laser Beam Welded Electrical Connections based on Artificial Intelligence

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Reliable transmission of electricity in battery cells and modules is indispensable in the course of the energy transition. However, state-of-the-art joining technologies like bolted or soldered connections reveal several drawbacks. According to VINARICKY [1], bolted joints show a force-dependent resistance, for instance. Soldering requires additional materials and suffers from low dynamic strength.

To overcome those disadvantages, laser beam welding seems to be a promising approach as it is a highly flexible and contactless joining process. Besides excellent joint properties, it is applicable to small assembly spaces and provides potential for lightweight construction. In addition, laser beam welding allows a controlled adjustment of certain properties like the electrical conductivity or the mechanical strength of the weld seam. SCHMIDT ET AL. [2] showed experimentally that the electrical conductivity can be set by an adjustment of the weld seam contour, see Figure 1. To assess the electrical conductivity, SCHMIDT ET AL. [2] derived the resistance factor as a dimensionless figure, for which the value of one is equal to the electrical properties of the raw material.

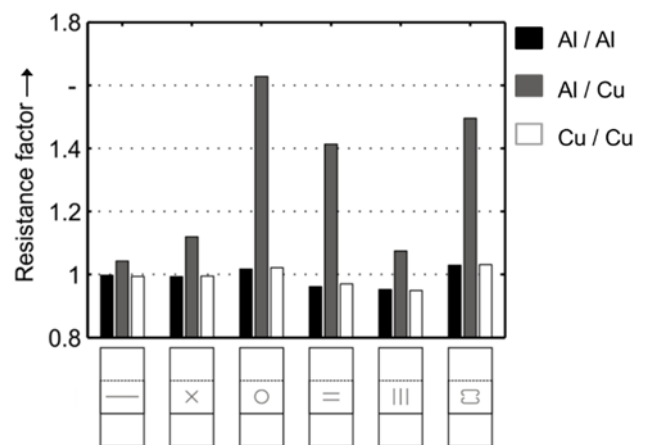


Figure 1: Electrical properties of different material combinations in overlap joint configuration for varying weld seam contours adapted from SCHMIDT ET AL. [2]

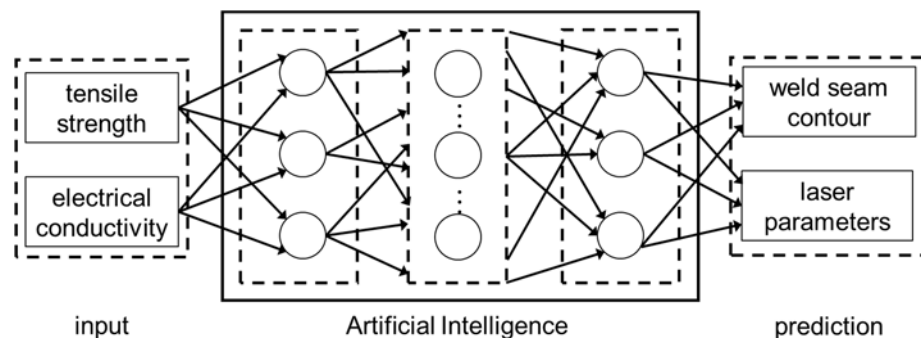


Figure 2: Prediction of the weld seam contour and laser parameters using Artificial Intelligence

strength, see Figure 2. Moreover, the capabilities and limitations of the investigated method based on Artificial Intelligence will be addressed.

- [1] Vinaricky, E.: Elektrische Kontakte, Werkstoffe und Anwendungen. 2. Auflage. Heidelberg: Springer, 2002. ISBN: 3-540-42431-8.
- [2] Schmidt, P.; Schweier, M.; Zaeh, M. F.: Joining of Lithium - Ion Batteries Using Laser Beam Welding: Electrical Losses of Aluminum and Copper Joints. In: LIA (Ed.): Proceedings of the 31st International Congress on Applications of Lasers & Electro-Optics (ICALEO). Anaheim, California, 23.–27.09.2012. Orlando: LIA pub., 2012, S. 915– 923.

EffSkalBatt: An efficient, scalable and sustainable stationary battery storage system design framework

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As the electromobility revolution led by battery electric vehicles takes off in earnest, an accompanying steep increase in lithium-ion battery (LIB) production volumes is imminent. A large number of batteries are expected to be available in the market, which can no longer fulfill stringent automotive standards, but which can still be put into service in other applications. The deployment of decommissioned automotive LIBs in second-life applications increases the total energy throughput of a battery over its extended lifetime, while simultaneously reducing the net ecological footprint of the technology over its lifecycle. Moreover, lack of standardization in the industry is a pressing concern for system engineers, which offsets the effect of price drop of batteries on account of higher design costs. The objective of the project EffSkalBatt is to establish a robust system design framework for new and second –life stationary battery energy storage systems to guarantee high system efficiency and scalability.

A holistic system modelling framework is to be developed over the duration of the project in tandem with the construction of a demonstrator, to enable validation and implementation of system concepts. Detailed characterization of components such as the power electronics, battery system, thermal and battery management systems is to be carried out to yield novel insights into the influence of these components at the system level.

Within the scope of the project, a target system is defined in order to identify interfaces and relations between different system components. The envisioned system concept is referenced to operational energy storage systems to ascertain the state-of-art. Key *performance* indicators are developed and applied to existing as well as future energy storage systems to quantify and benchmark their performance in various grid-related application scenarios.

In this contribution, we show the first results of an efficiency analysis carried out to ascertain the influence of power electronics topologies, their load distribution strategies, cell parameters such as internal resistance as well as the suitability of a particular application to a given system configuration. Also presented are key performance indicators and their applicability to future system concepts.

Energy self-sufficiency in small to medium sized breweries

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Compared to other sectors in the food and drink industry, brewing of beer is considered an energy-intensive process. In Germany, breweries are faced with a shifting energy market (German Energy Transition) as energy prices tend upwards. Furthermore, the majority of breweries are dependent on fossil fuels and third-party electricity supply.

To address the potential of renewable energies, a feasibility study on energy self-sufficiency in small to medium-sized breweries (SMBs) was conducted. In contrast to previous work, the study considers energy efficiency, renewable energies and on-site energy generation simultaneously to investigate self-sufficient energy systems.

Within the framework of the Energy Value Stream Method, a top-down approach was applied for hierarchically structuring a SMB in Bavaria, Germany, followed by a holistic analysis of energy and material flows. The energy demand at unit level (e. g. mash tun) is then derived using a MATLAB/Simulink model. To investigate self-sufficient energy systems in SMBs, a three-step procedure is proposed. In this context, a material flow simulation is applied to generate electricity and heat load profiles. These profiles are then used to develop various scenarios for sustainable on-site energy generation. For scenario evaluation, a multi-attribute decision analysis is adapted to address economical, technical, ecological and social aspects.

For SMBs a degree of energy self-sufficiency of 0.38 (ratio between on-site and third-party supply) can be achieved using state-of-the-art energy supply technologies. This ratio can be increased up to 0.73 by integrating electrical energy storage systems, while a ratio of 1.00 is achievable but economically inefficient.

Synthesis of Polythiophene Derivatives and Graphene Oxide for Organic Solar Cells

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Polythiophene derivatives and graphene oxide are used as electron donor and electron acceptor respectively in organic solar cells. The synthesized molecules are electrically conductive, contain no heavy metals / heavy metal complexes and require no doping which makes them environmentally friendly. They are compared to conventional inorganic semiconductors flexible, transparent, light weight and have low energy costs per surface [1]. Special applications of these cells are in glass facades or in clothing, where regular silicon technology cannot be used. For further progresses in organic electronics the synthesis of new air-stable organic materials is therefore essential to create new sustainable materials for organic solar cells.

The homopolymers poly(3-hexylthiophene) (P3HT), poly(3-thiopheneacetic acid) (P3TAA), poly(3-thiopheneethanol) (P3TE) and the related copolymers are prepared starting from the respective monomer units by chemical oxidative polymerization. Due to the different substitutions of the thiophene ring different solubilities in organic solvents and water are achieved. Polymers with acetic acid groups (-COOH) like P3TAA or hydroxyl groups (-OH) of P3TE are for example very good soluble in polar solvents like acetone compared to P3HT, which is only soluble in more hazardous solutions like chlorobenzene.

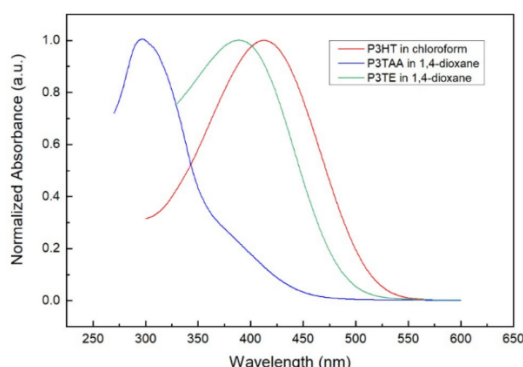


Figure 1: Absorption spectra of polymers in solution

Figure 1 shows the absorption spectra of P3HT, P3TAA and P3TE in solution with peaks appearing at 297, 391 and 414 nm respectively. Since the monomer peaks appear all at 234 nm the polymers are all redshifted compared to the respective monomers, which indicate the successful synthesis of the polymers. The results show that the polymer backbone therefore increased with polymerization, with P3HT being the polymer with the longest mean conjugation length, followed by P3TE and then P3TAA.

The polymers are used together with synthesized graphene oxide as active layer in organic solar cells. Graphene oxide is compared to graphene liquid processable, has a higher dispersibility in organic solvents and water and forms more homogeneous layers [2]. These properties result mainly due to the functionalization of graphene with polar groups (carboxyl or hydroxyl). Figure 2 shows for graphene oxide additional infrared vibrations between 3700-2500 cm^{-1} and 1703 cm^{-1} which can be attributed to hydroxyl and carbonyl group vibrations respectively and indicate the successful synthesis of the nanomaterial.

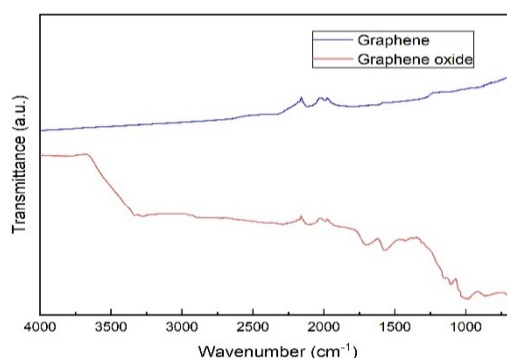


Figure 2: Infrared spectra of graphene and graphene oxide.

References:

- [1] J. Li., S. Kim, S. Edington, J. Nedy, S. Cho, K. Lee, A. J. Heeger, M. C. Gupta, Y. T. Yates, Sol. Energ. Mat. Sol. Cells. 95, 1123-1130 (2011)
- [2] V. V. Neklyudov, N. R. Khafizov, I. A. Sedov, A. M. Dimiev, Phys. Chem. Chem. Phys. 19, 17000 (2017)

The interactive eRoad Webmap

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Throughout the project eRoad: Pisek-Deggendorf, the goal was to foster the adoption of electro mobility. Politics as well as research institutions are in common that one of the most important factors hereby is the establishment of a comprehensive charging station infrastructure which is the reason why the project was mainly focused on this.

As Bavaria is rushing forward with own incentive programs to support this development, Lower Bavaria is used as a role model for the neighboring federal state South Bohemia in Czech Republic. To assess the actual demand for energy in the individual electric transportation, analyses were executed on basis of

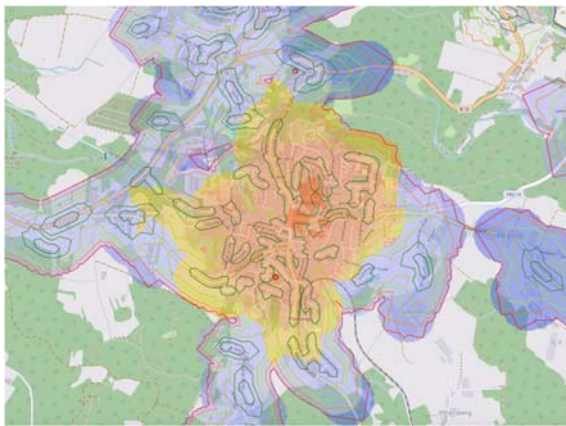


Figure 1: Example of Electric Vehicle Charging Demand and Walking Distances from POIs in Freyung, Germany

Points of Interest (POIs). For that, OpenStreetMap POIs were split into the four different categories living, work, recreation and shopping. Those categories do not only serve to allocate the POIs accordingly, they also include the individual time spent at such places. It is assumed that the timespan spent at a POI is one important parameter to define the electric charging demand, thus it was one crucial factor to be considered in the calculations. Another indicator for electric vehicle demand is the walking distance between the possible charging station location and the actual POI. The time spending as well as the walking distances were furthermore diversified into four demographic classes, ranging from young agers (18-29) to silver agers (65+). The different classes depict the varying times spent per POI category and age as well as the distinctive walking distances, people are willing to take to get from the parking space to the destination.

After the demand was spatially distributed and calculated with the input data as described above, the renewable energy generation sites nearby were assessed to see how the charging stations can be fed by low carbon renewable energy sources. The next place, where electric energy is generated can on the one hand help to release pressure from the electric grid and provide onsite energy production for possible charging stations. On the other hand, it can support to increase the share of used renewable energy sources for the electricity of e-vehicles. Only by using renewable energy sources, the possibility to really drive CO₂ friendly is given and should therefore be pursued.

An online interactive web map was created in order to let regional planners, policy makers and the interested public find the best place for an electric vehicle charging station. The web map allows to review current and possible future electric energy demands for e-vehicles and where they probably will be needed, walking distances from POIs, the distance one can drive with a common electric vehicle from existing charging stations and the currently existing renewable energy generation sites. It is furthermore possible to draw lines and polygons to assess sizes and locations as well as to pin certain spots on the map individually. The web map is accessible via internet at: <https://eroad.th-deg.de>.

Printed active layers for organic solar cell application

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In the past few decades, organic solar cells (OSCs) have received great progresses through novel organic materials. With the advantages of highly tunable molecular energy levels and light absorption spectra, OSCs employing non-fullerene accepters have made breakthroughs of efficiencies over 16% [1]. Furthermore, the advantages of large-area processing technique, such as slot-die printing fabrication, makes non-fullerene

OSCs very commercial attractive as a cost-effective solution. However, the achieved best efficiency remains behind than that of traditional silicon solar cells, which demonstrates the needs of intensive investigation [2]. The morphology of active layer has great influence on the organic solar cell performance, thus, tuning the morphology by adding functional additive is a feasible strategy to achieve decent efficiency. In the present work, the bulk heterojunction (BHJ) solar cells were fabricated with medium-bandgap donors (PBDB-T-2F) and non-fullerene acceptors (IT-M) via slot-die printing to enable industrial scale up-scaling. The molecular structure of the materials and

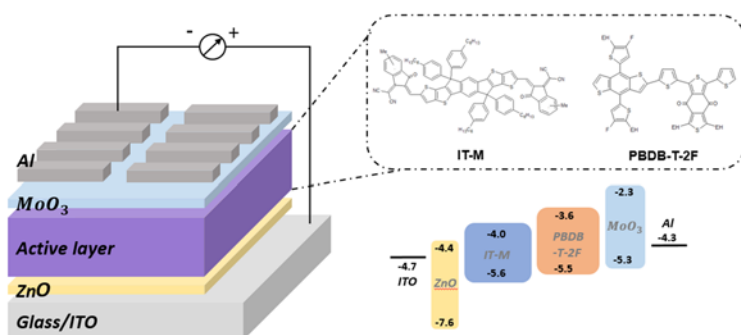


Figure 1. Schematic diagram of the bulk heterojunction (BHJ) solar cells, donor (PBDB-T-2F) / acceptor (IT-M) molecules, and the energy level diagram of the system.

invert BHJ solar cell geometry are shown in Figure 1. When the light is absorbed in the active layer, excitons are generated in the active layer. Meanwhile, the excitons are dissociated into electron-hole pairs and transferred to the corresponding electrodes eventually. Because of proper working function and high transmittance, ZnO and MoO₃ are quite promising material for hole blocking layer and electron blocking layer, especially for BHJ solar cells.

The active layers consisting of PBDB-T-2F:IT-M mixture are printed in the air condition at room temperature with a printing speed of 5mm/s. By adding different ratios of 1,8-diiodooctane (DIO) additive, the photoluminescence properties of active layers and the neat thin films are shown in Figure 2a. As for the active layer thin films, the PL spectrums locate in the range of 700-900 nm with a 550 nm excitation wavelength.

The UV-vis absorption spectrum of the thin films of the donor and the acceptor are depicted in Figure 2b. PBDB-T-2F is a medium band gap polymer donor for solar cell of which absorption mainly lies in the range of 300-700nm. And the absorption spectra of IT-M is mainly located in the range of 500-800 nm, which is complementary to that of PBDB-T-2F. For systematic understanding of DIO additive influences on the active layer morphology, various measurements will be carried out, such as atomic force microscopy (AFM), scanning electron microscopy (SEM), and grazing incidence small/wide angle X-ray scattering (GISAXS / GIWAXS).

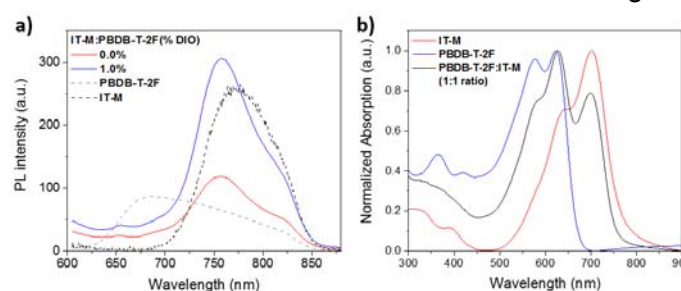


Figure 2. The photoluminescence intensity of active layers with various DIO additive ratios and the absorption spectrum (UV-vis) of IT-M and PBDB-T-2F

References

- [1] Fan B, Zhang D, Li M, Zhong W, Zeng Z, Ying L, et al. Achieving over 16% efficiency for single-junction organic solar cells. *Science China Chemistry*. (2019)
- [2] Wei Li, Jinlong Cai, Yu Yan, Feilong Cai, Sunsun Li, and Tao Wang, *Sol. RRL*, 2, 1800114 (2018)

Towards a Sustainable Energy Mix: Ecuadorian case

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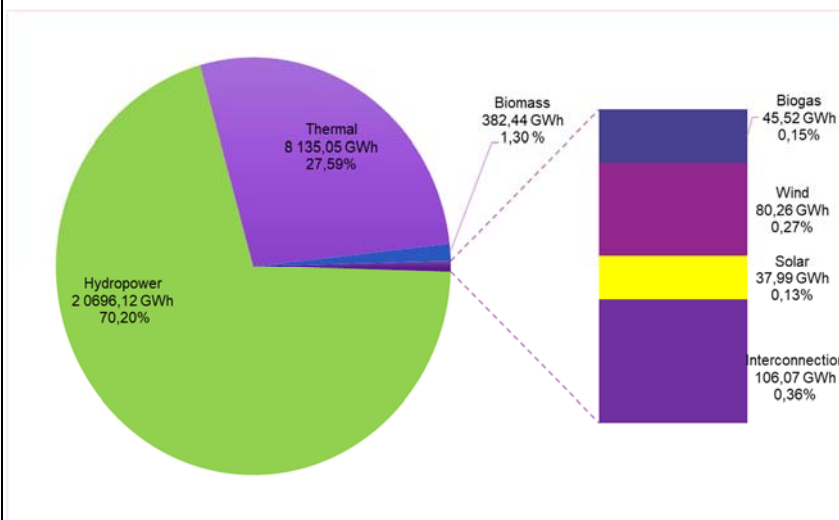


Figure 1: Ecuadorian electricity mix in 2018

Ecuador, as many other south American countries, exports raw materials based on natural resources, such as bananas, cacao, flowers, sea products, and of course oil, to import final products. In fact, Ecuador is the fifth oil exporter country, and the third one with the biggest oil recoverable reserves in Latin America [1]. Since the first oil barrel arrive from the amazon to the coast region in Ecuador, the power sector has been dominated by thermal plants, however through the history that scenario has changed with the renovation of the electric public sector institutions and more important, the continuous change in the energy policies.

One of the biggest changes occurred in 2007, when the Ecuadorian government decided to transform the national productive mix, and with it, the change of the energy mix in order to use the renewable potential for electricity generation, and after a great investment in the power sector, in 2018 hydropower was consolidated as the most important energy supply in Ecuador, followed by thermal, and the other energy supply resources, except for biomass, contributed with less than one percent to the energy mix (see Figure 1) [2]. The energy policies have been favorable for the hydro energy developing, however it is evident the dependence on just one natural resource and the lack of incentives for the non-conventional renewable energy.

This research will take into account the social and environmental aspects which has to be considered in countries which delicate ecosystems, and where the construction of big energy projects affects the surrounding areas. This study looks for a sustainable and optimal energy mix in which the non-conventional renewable energies take part of the electricity generation, and avoid only one resource dependence in a rich of natural resources country, as Ecuador.

Key Words: Ecuador, energy mix, hydropower, urbs.

- [1] World Energy Council. "Energy Resources in Latin America & The Caribbean". 2015. Available: <https://www.worldenergy.org/data/resources/region/latin-america-the-caribbean/oil/>. [Accessed 14 March 2019].
- [2] Agencia de Regulación y Control de Electricidad, ARCONEL, "Balance Nacional de Energía Eléctrica". 2018. Available: <https://www.regulacionelectrica.gob.ec/balance-nacional/>. [Accessed 11 March 2019].

Identification of Active Electrocatalytic Sites Using Electrochemical Scanning Tunneling Microscopy

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The advent of the “hydrogen economy” would provide an abundant, sustainable and worldwide accessible energy system. However, in order for such electrochemical energy provision devices to become competitive in contributing to new environmentally friendly energy production schemes, suitable catalysts have to be developed, in this study in particular for the hydrogen (HER) and oxygen evolution reaction (OER). The activity of such a catalyst, *i.e.* the increase of the reaction rate in the catalyst’s presence, is in turn highly dependent on the electronic structure of specific surface sites that offer optimal binding of reaction intermediates. Thus, the reactions take place at these so-called “active sites”. The geometric structure of optimal active sites is commonly predicted by Sabatier-type volcano plots. Combining theoretical predictions with a technique that is able to directly identify and monitor these sites in-situ while the reaction is taking place would therefore be a powerful tool to advance the performance and rational design of catalysts.

Here we demonstrate the potential of a conventional scanning tunneling microscope (STM) to spatially map and in-situ identify active sites on a catalyst’s surface with resolutions down to the nanometer or even atomic scale. In general, the recorded tunneling current depends on several factors such as tip-sample distance, surface electronic structure and tunneling medium. As shown in Figure 1, reactants and products ad- and desorbing on and from the surface present in the tunneling gap, change the composition of the medium, and thus have an influence on the tunneling current. By monitoring relative changes in the tunneling current, an increased noise level was detected over active centers, confirming electrochemical STM (EC-STM) as a powerful tool to determine the position of active sites.

EC-STM was employed on Iridium (Ir) oxide for the OER and on highly oriented pyrolytic graphite (HOPG) for the HER. As can be concluded from the noise level in Figure 2, the active sites on the Ir oxide seem to be equally distributed across the surface whereas on HOPG the active sites are located at the step edge.

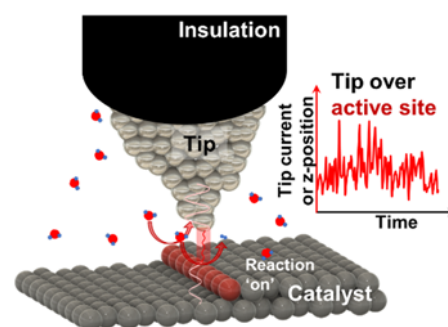


Figure 1: Concept of EC-STM.

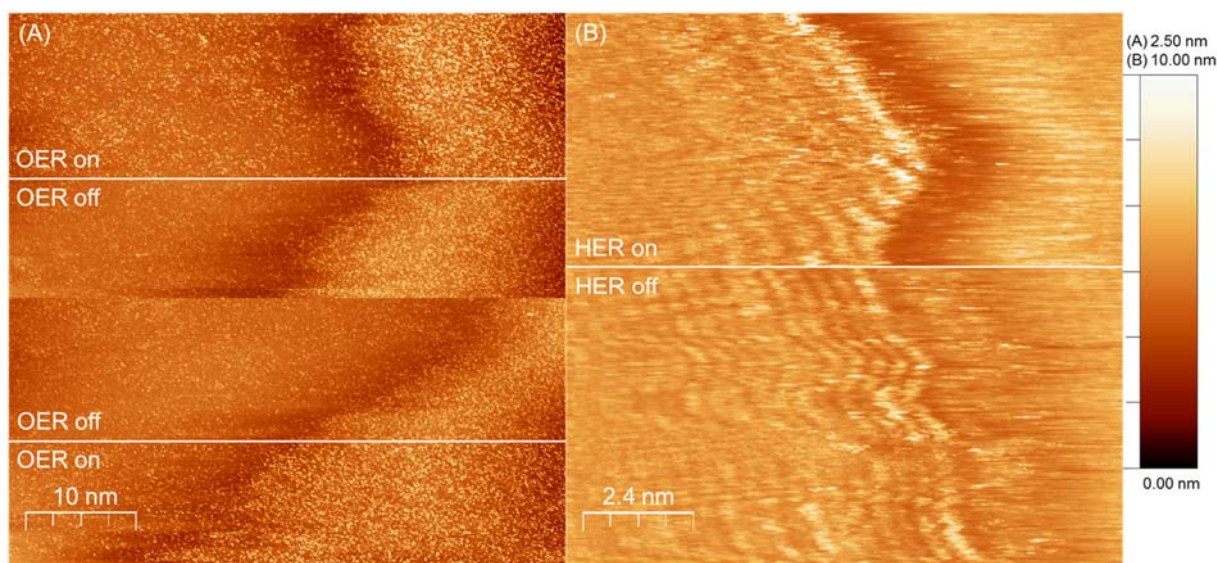


Figure 2: EC-STM measurements on (A) Ir oxide for OER and on (B) HOPG for HER.

A Comparative Study of Platinum-Ruthenium Core-Shell and Platinum-Alloy Catalysts' Activity Towards the Hydrogen Oxidation Reaction in Alkaline Media

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With an increasing demand for renewable energies, the use of hydrogen as a fuel is one suitable alternative to fossil fuels. For automotive applications, major companies like Toyota, Honda and Mercedes focus their research in PEMFCs (proton exchange membrane fuel cells) and the first commercial FCVs (fuel cell vehicles) have been on the market for years.^[1] However, these cars, such as the model 'Mirai' by Toyota in 2014 with a starting price of \$57.500 are still much more expensive than a typical family car.^[2] To introduce affordable FCVs into the market, a major challenge in the production of such vehicles is to cut down the amount of expensive Pt used as the catalyst, while still maintaining or even increasing the performance. To tackle this issue, Pt could be alloyed with a less expensive metal or a more sophisticated catalyst design, such as core-shell structure, could be used, where the core is the less expensive metal. Pt is used at both the anode and the cathode sides for the hydrogen oxidation reaction (HOR) and the oxygen reduction reaction (ORR) respectively. In a long-term perspective and due to the sparse deposits of Pt, it is in the best interest to lower the amount of Pt used in both anode and cathode sides. In this presentation, various carbon supported catalysts, including Pt/C, Ru@Pt/C core-shell, PtRu/C alloy and PtNi/C alloy, were electrochemically tested using the RDE (rotating disc electrode) technique in acidic and alkaline electrolytes. The catalysts were compared with respect to their HOR/HER (hydrogen evolution reaction) activity. Pt/C, Ru@Pt/C and PtRu/C were synthesized using the polyol reduction method. The catalysts were tested for their cyclic voltammogram (CV) and CO strip in acidic and alkaline media. Further, the HOR/HER activity was tested exclusively in alkaline media. The reliability of both the synthesis and the measurement methods were confirmed by the investigation of the self-made Pt/C reference with an HOR/HER activity in good agreement with literature values.^[3,4] Furthermore, the activity of the Ru@Pt/C catalyst aligns well with a previous study, proving that the upscaling of the catalyst was successful.^[3] Overall, the order of the HOR/HER specific activity was determined to be Ru@Pt/C > PtRu/C > PtNi/C > Pt/C, with Ru@Pt/C having the highest activity at $i_{0\text{surface}} = 1.71 \pm 0.2 \text{ mA/cm}^2_{\text{metal}}$.

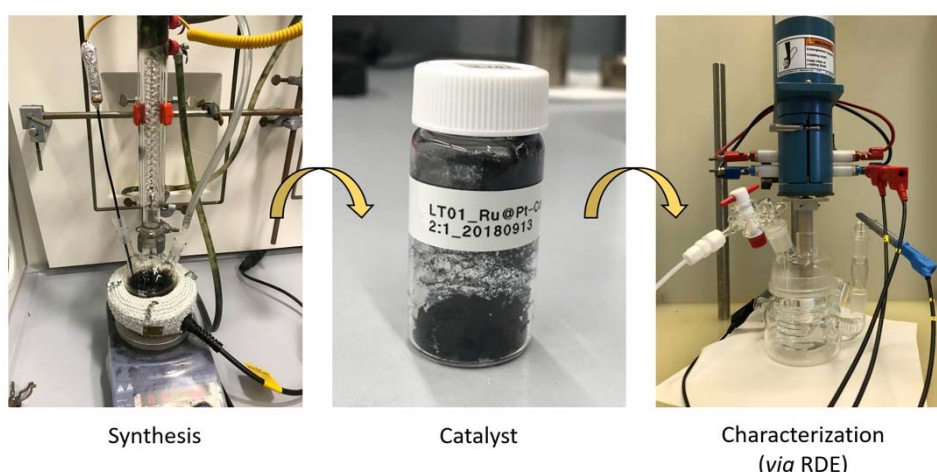


Figure 1: Experimental procedure of this work. The catalysts were synthesized via the polyol reduction method and were then characterized using the RDE technique under acidic and alkaline environments (acidic RDE setup shown here).

- [1] R. E. Rosli, A. B. Sulong, W. R. W. Daud, M. A. Zulkifley, T. Husaini, M. I. Rosli, E. H. Majlan, M. A. Haque, *Int. J. Hydrogen Energy* **2017**, 42, 9293–9314.
- [2] T. Yoshida, K. Kojima, *Interface Mag.* **2015**, 24, 45–49.
- [3] J. N. Schwämmlein, B. M. Stühmeier, K. Wagenbauer, H. Dietz, V. Tileli, H. A. Gasteiger, H. A. El-Sayed, *J. Electrochem. Soc.* **2018**, 165, H229–H239.
- [4] S. St. John, R. W. Atkinson, R. R. Unocic, T. A. Zawodzinski, A. B. Papandrew, *J. Phys. Chem. C* **2015**, 119, 13481–13487.

Structure-Activity Correlation by Soft-XAS Analysis of Carbon-Supported $\text{Fe}_x\text{Zr}_{1-x}\text{O}_{2-\delta}\text{N}_y$ as ORR catalyst for PEMFCs

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One of the major hindrances to mass commercialization of low-temperature proton-exchange-membrane fuel cells (PEMFCs) is the considerable amount of expensive Pt required, mostly at the cathode side, where the oxygen reduction reaction (ORR) takes place. [1] On the other hand, the challenges for Platinum-Group-Metal free (PGM-free) ORR catalysts are an activity approaching that of Pt and a long-term operational stability in the strong acidic environment of a PEMFC.

Low-cost metal-nitrogen-doped carbons (M-N-Cs, M = Fe, Co) currently are the most promising PGM-free catalysts in terms of activity requirement, but they still face stability issues in acidic environment [2, 3]. On the other hand, valve metal oxides need a significant improvement in ORR activity but they are very promising in terms of their stability during PEMFC operation. [4, 5]

After our previous studies on carbon-supported Fe-substituted nanometric ZrO_2 [6, 7], some questions were left unanswered, i.e., the structural reason for its optimal activity and the role of nitrogen. To answer these questions and further understand the structure of the most active catalyst in RDE, we analyzed nanometric $\text{Fe}_x\text{Zr}_{1-x}\text{O}_{2-\delta}$, synthesized at different Fe at% and heat treatment temperatures, using X-ray powder diffraction and soft X-ray absorption spectroscopy at the O K-edge, Fe L-edge and N K-edge. We correlated the structural information obtained with the activity measured with a rotating disc electrode (RDE) setup.

With these data we aim at showing how substituents and temperature affect oxygen chemical environment, Fe oxidation state and N content/coordination, thus providing more insight to the active catalyst structure.

References:

References:

[1] A. Kongkanand and M. F. Mathias, J. Phys. Chem. Lett. 7 (2016) 1127-1137.

[2] M. Lefèvre, J. P. Dodelet, ECS Transactions 45(2) (2012) 35-44.

[3] B. Piela, T. S. Olson, P. Atanassov, P. Zelenay, Electrochimica Acta 55 (2010) 7615-7621.

[4] A. Ishihara, S. Yin, K. Suito, N. Uehara, Y. Okada, Y. Kohno, K. Matsuzawa, S. Mitsushima, M. Chisaka, Y. Ohgi, M. Matsumoto, H. Imai, K. Ota, ECS Transactions 58 (2013) 1495-1500.

[5] T. Mittermeier, P. Madkikar, X. Wang, H. A. Gasteiger and M. Piana, J. Electrochem. Soc. 163 (2016) F1543-F1552.

[6] P. Madkikar, T. Mittermeier, H. A. Gasteiger, M. Piana J. Electrochem. Soc. 164(7) (2017) F831-F833.

[7] P. Madkikar, D. Menga, G.S. Harzer, T. Mittermeier, A. Siebel, F.E. Wagner, M. Merz, S. Schuppler, P. Nagel, A.B. Muñoz-García, M. Pavone, H. A. Gasteiger, M. Piana, J. Electrochem. Soc. 166(7) (2019) F3032-F3043.

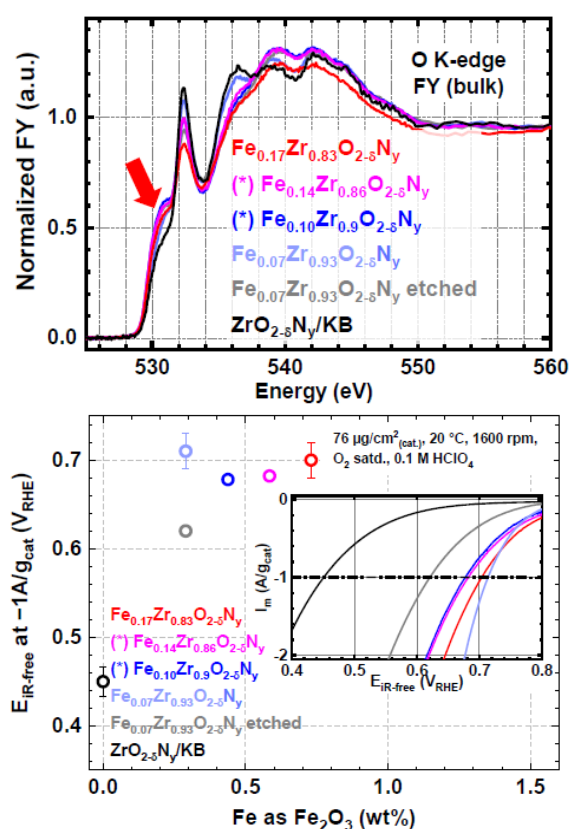


Figure 1: (top) O K-edge spectra of samples synthesized at different Fe at%. (bottom) ORR activity in RDE of samples synthesized at different Fe at%.

Capture and Control of Material Flows and Stocks in Urban Residential Buildings

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To promote the circular economy and resource efficiency in the construction industry, information on material flows (e. g. raw materials, building materials, waste, etc.) and the material composition of the building stock is needed. Through this knowledge for example, the occurrence of potential secondary raw materials (e. g. recycled building materials) can be forecast. Furthermore, systematic recovery and utilisation strategies can be identified and further developed (material flow management).

This work describes the development of a holistic and dynamic material flow model for the determination of the material composition of the housing stock (material cadastre) and the associated material flows triggered by urban housing. Material characteristics at building-, component- and material level were combined with geometric data from 3D city models to represent the current condition. This information serves as the basis for further calculations (e. g. proportion of recyclable masses, construction waste, system losses, etc.).

The model developed in this work was validated on the basis of the district of Munich / Freiham, one of the largest urban developments in Germany. It has been shown that around 2.2 million tonnes of building materials are currently bound within the residential buildings of the focus area. Of these, around 48 % are concrete and 24 % bricks. Approximately 5 % of the examined stock consists of metals, with a current equivalent value of approximately € 20.4 million. About 50 % of the total mass is bound in apartment buildings of the age groups 1958 - 1968 (31 %) and 1969 - 1978 (19 %).

Based on the case study, the potentials of mass balances (self-sufficiency of urban spaces with materials) could be demonstrated. Under the chosen conditions, it is possible to achieve a self-sufficient supply of steel from about 2036 for the construction of housing within the focus area and from about 2031 with recycled aggregate for the production of recycled concrete.

By knowing the whereabouts (geographical and temporal occurrence and demand) of materials, a targeted use of secondary raw materials from the building stock can be enforced. Systematic material flow management (e. g. high-quality on-site recycling) in urban areas therefore has a high potential to increase the share of secondary resources and to reduce the use of primary resources and transports. In order to put these measures into practice, a common data space (e. g. continuously updated database on material composition of buildings) is needed to optimize the exchange of information between the different actors along the value chain and to coordinate the supply and demand for materials.

Environmental impacts of buildings on basic human needs

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Starting point and purpose

Since 1987, the aim of „Sustainable development“ has been to ensure the basic human needs of future generations. The precondition for the preservation of human existence is a working environment with all its functions, ecosystems, system services and resources. A closer look at environmental impacts shows that the construction industry makes a significant contribution to the consumption of resources and the production of waste and emissions. Based on those facts, this study aims to examine the environmental impacts of a building on the basic human needs. The challenge was to elaborate and qualitatively evaluate the single correlations and systemic effects.

Approach and result

Through assigning the sustainable development goals to the basic human needs and higher needs (Basis Maslows pyramid of desires) and the assignment to the three sustainability dimensions was clearly evident, that every sustainable target with ecological orientation serves the assurance of the basic human needs. Based on this framework the 17 German sustainable development goals were restricted to the 5 environmental goals. The methodology, as seen in Figure 1, presents the connections and enables a

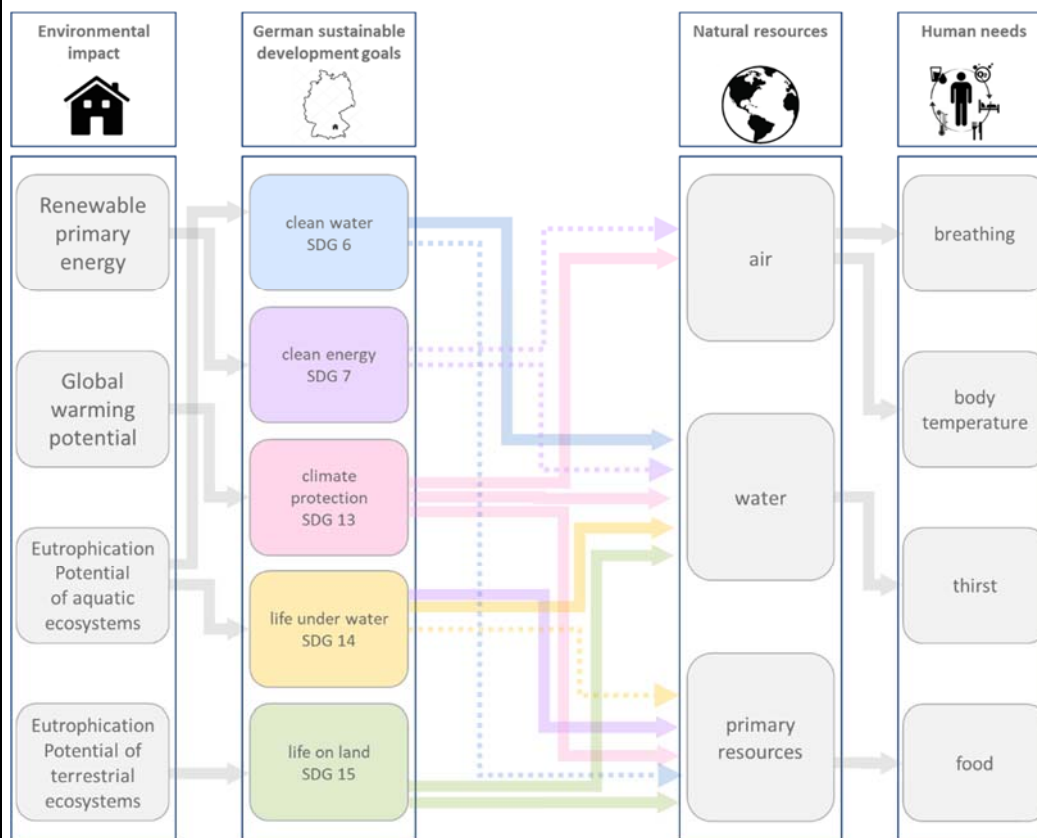


Figure 1: Relation of environmental impact of buildings to the human needs

quantitative evaluation is not yet possible. In order to further promote sustainable buildings and its effects on basic human needs a key finding of this study is, that more research has to be carried out in order to be able to fully quantify all the ecological impacts.

a qualitative evaluation of the results. A closed-circuit result from the summary of all commonalities and surfaces of the single system parameters, whereby the influence of the environmental impacts of a building is explained. Consequently, a sustainable and in particular conscious construction is imperative in order to enable future generations to ensure their basic human needs. Small changes in a planning process, such as a choice of more sustainable materials, can have a relatively high positive impact on the environment. A major issue though is the limited and one-sided data available, hence a holistic

Energy, Room Climate and User Behavior Monitoring of an Office Building with Three Different External Wall Constructions

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In order to increase energy efficiency and promote renewable energies, newly constructed buildings must comply with the current German energy saving ordinance (EnEV). A challenging task during the planning stages of a building is to deal with the uncertainties between the predicted energy demand and the real energy consumption during the operation. These uncertainties derive from different generic assumptions in the German energy saving ordinance e.g. regarding the material composition of building envelops (heat storage capacity) and the user behavior (generic user profiles). Such uncertainties can lead to an oversizing of the building services and/or the thermal building envelope. Hence, the question that arise is: How does the planned building behave in terms of energy consumption and indoor climate in reality? In order to answer this question, the objective of this study is to identify and analyze the differences between the estimated energy demand and the actual energy consumptions of an office building, built in 2016, in Regensburg, Germany.

In this case study an extensive building monitoring was carried out during the years 2017 and 2018. With the way the building is constructed, see Figure 1, one can also get in-depth insight in how the material composition of external wall affects the energy consumption and how the indoor climate is affected by the ambient climate. Examining the total energy demand for heating, the EnEV predicts an annual energy demand of 39,937 kWh/a. By contrast, the measured energy consumption for heating amounts to 36,428 kWh in 2017 and 36,175 kWh in 2018. It becomes apparent, that the actual energy consumptions is about – 10% lower than what was predicted according to EnEV. In the floor specific evaluation, it can be seen that the energy consumption for heating in the first floor is significantly lower compared to the ground floor and the second floor. This can be explained by the fact that the floor and ceiling adjoin heated parts of the building. Looking at the energy demand for cooling it must be noted that no cooling was considered in the calculation according to EnEV. However, in reality there is a demand for cooling measurements, which amount to an energy consumption for cooling to 5,646 kWh in 2017 and 9,688 kWh in 2018. Considering heating and cooling the total energy consumption amounts to 42,074 kWh in 2017 (+ 5% EnEV) and 45,863 kWh in 2018 (+ 15% EnEV).

In addition, the current research focuses on evaluating the user behavior data with machine learning algorithms. The aim is to identify how the user behaves in certain boundary conditions and its effects on the energy consumption. The findings can then be used to improve and validate thermal building simulations.

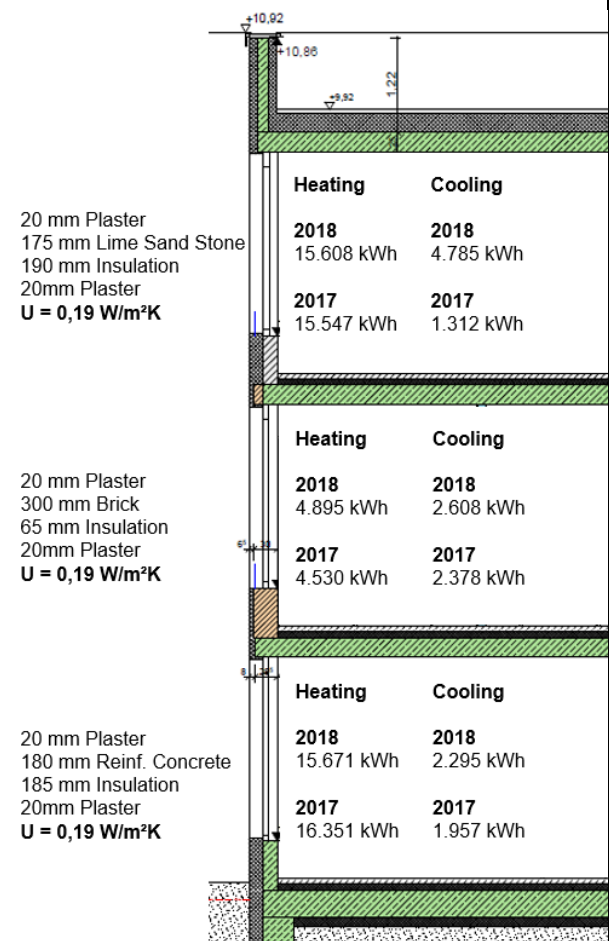


Figure 1: Cross Sections of the building showing the material compositions and the energy consumptions for heating and cooling

Data Deficits in the Life Cycle Assessment of Buildings

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In regards to the current development of stricter requirements to further increase the energy efficiency of buildings, the relative share of the, in the building materials embedded energy compared to the total life cycle based energy demand rises. The total life cycle energy demand includes the extraction of resources, material production, transportation, use and end of life of a building. Hence, a Life Cycle Assessment (LCA) is needed in order to identify and evaluate the total energy demand and environmental impacts over the whole life cycle of buildings. Since reliable data is necessary to perform a LCA the findings of this research refer to the question about the influence of data deficits on the results of a building LCA. Particularly important in this context is i.a. the environmental indicator Global Warming Potential (GWP) that is considered in particular in the scope of this research.

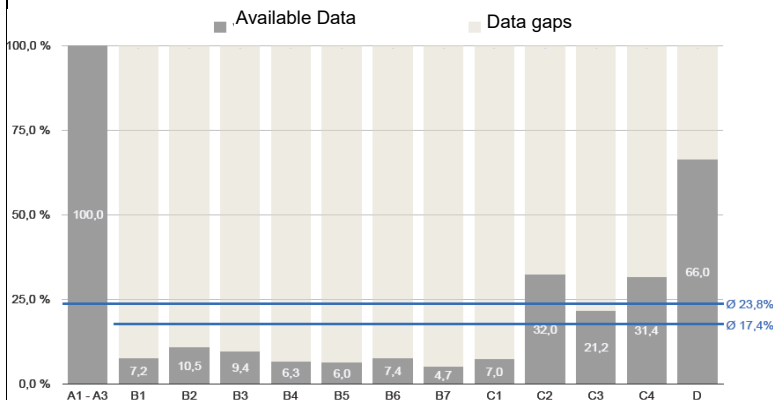


Figure 1: Percentage of declared data records per life cycle module of ÖKOBAUDAT 2017

In this study, the freely accessible platform ÖKOBAUDAT, which is commonly used for building LCA, represents the database. An analysis of the data source ÖKOBAUDAT (as of 2017) shows (see Fig. 1), that about 24 % of the data records are declared in an average data module. According to DIN 15978 and DIN 15804 the complete building life cycle is defined by phases A1 to D. However, ÖKOBAUDAT data records only have to contain a declaration of the manufacturing phase (A1-A3) in order to be included in the database. This justifies the incomplete nature of the available data sets. This justifies the incomplete nature of the available

data sets. In order to determine the actual influence of this deficient data situation on the estimation of potential environmental impacts, two LCAs of an office building, as case study, are performed in two different ways. At first a "Simple Life Cycle Assessment", which uses solely data from ÖKOBAUDAT with no measures taken to eliminate data deficits and secondly a "Detailed Life Cycle Assessment" using a methodology to eliminate data deficits. The methodology was developed at the Institute of Energy Efficient and Sustainable Design and Building of the Technical University of Munich. Based on the principle of transparency, it is applied to the case study.

The subsequent comparison of both LCA results shows clear differences in the calculated potential environmental impacts. As seen in Figure 2, the total GWP ($\Sigma A-C$)

amounts to about 137.000 kg CO₂-eq. for the Simple LCA and 266.000 kg CO₂-eq. for the Detailed LCA. This significant difference (about 94 %) shows the importance to take actions to eliminate data deficits since they can lead to inaccurate LCA calculations and to incorrect measures during the planning phases of buildings.

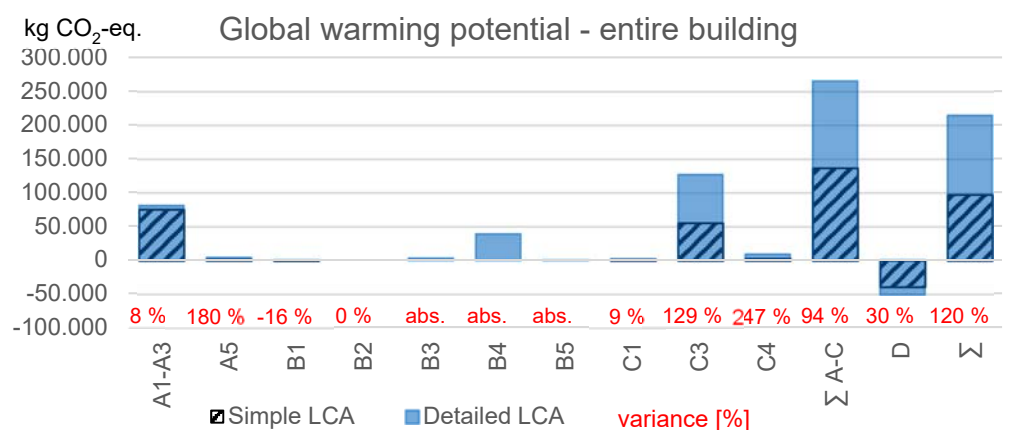


Figure 2: Comparison of balance sheet results for GWP in the entire construction of the building

Solar activated envelopes in district context – design and assessment concepts

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The decarbonization of the building stock is essential for achieving the climate protection targets in Germany and is not conceivable without intensified utilization of renewable energies, in particular solar energy. As urban roof areas for solar installations are limited, facades become relevant for energy activation, requiring high architectural quality in order to achieve universal acceptance. Due to rising temperatures especially in urban spaces, strategies for climate adaptation, e.g. by enhanced greening of urban districts, are gaining in importance as well.

Thus, the research project Cleanvelope aims to investigate the synergy potential of solar energy use as a climate protection strategy and greening as a climate adaptation strategy in building envelopes without compromising the architectural quality of the built environment. Attractive design concepts at a district level accompanied by application guidelines will reduce existing reluctance to apply solar energy systems in building facades due to aesthetical and warranty reasons.

So far, renewable energy production in district energy concepts is mainly limited to solar roof installations. Due to increased complexity and costs, solar energy activation of facades in an aesthetic way is solely considered in a limited number of new constructions, even if the existing building stock offers a wider solar potential. Moreover, synergies between solar energy generation and building greening scientifically nearly remain unnoticed.

The innovative approach of Cleanvelope is a holistic analysis of energy activated building envelopes of the urban building stock while taking local building culture into consideration. By using a bottom-up approach, solutions for integrating solar energy in urban residential districts with high architectural quality will be developed and synergies between energy activated building envelopes and façade greening will be analyzed. The analyses take place at district level in order to develop coherent design concepts for selected residential areas and to promote the use of solar energy at large scale. The results will be integrated into urban development tools and thus offer support in taking urban planning decisions.

To quickly identify high performance solutions for a wide number of different urban settlement typologies, an assessment system will be developed, taking into consideration competing installations on building envelopes, synergies between energy activated building components and green areas, as well as the architectural appearance and technical quality of the redesigned facades. As part of the project, students attending a master's course at the Technische Universität Nürnberg will conceive first design solutions for building envelopes including solar energy production and building greening. Hereafter, the assessment approach as well as further refined design solutions will be discussed in workshops with experts like architects and urban planners and subsequently revised based on the workshops' recognitions.

At the MSE Energy Colloquium, the assessment system will be presented and the students' designs will be visualized by means of renderings and physical models. As a prospective result, a systematic application catalogue containing best-practice solutions will aim at providing new impulses for practical implementation and stimulating the large-scale solar energy activation of the urban building stock and notably its facades. Additionally, simulations will quantify synergy effects of solar activation and building greening.

This project is sponsored by the Bavarian Ministry of Science and the Arts in the context of Bavarian Climate Research Network (bayklif).

Investigating the dynamics of material composition of buildings during their lifecycle

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Every building consists of building materials which can potentially be reused during or at the end of its lifecycle in order to save natural resources and energy. The planning of such long-term strategies for sustainable resource usage requires detailed knowledge about the used quantity of building material, its characteristics and quality.

For older buildings, specifications regarding their material composition are often insufficient and documenting them may prove hard because of missing or flawed documents. Furthermore, due to their long existence, frequent restorations can take place which change the composition of materials in those buildings.

This work examines the change of material composition of buildings over a period of 80 years. To this end a residential complex situated in Munich is studied in detail. Information about used building material and its change is gathered by analyzing documents from archives and local measurements. In doing so, proportions of mineral materials, ferrous and non-ferrous metal, gypsum, timber, plastic, insulation material, and glass are examined.

The results of this work give an explanation about the change of material quantities and types for distinct stages during the lifecycle of a building.

Development of a radiant heating and cooling model for the implementation of sustainable buildings

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This study aims to investigate the impact of building services system on the energy demand of a building, taking account of a strict building standard and energy supply concepts based on renewable energies. A building zone is modelled in TRNSYS regarding a sustainable heating and cooling energy production by radiative solar heating and cooling in combination with thermal storage tanks (Figure 1).

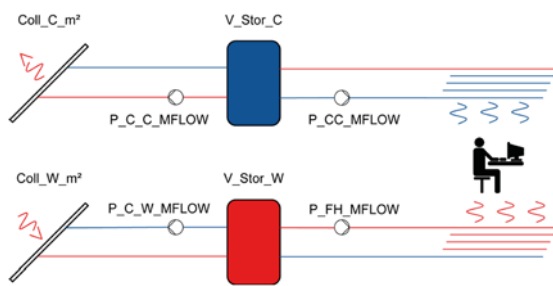


Figure 1: Scheme of system and building technology

The control loop for heating the building consists of a sensitive thermal storage tank and a thermal collector surface for energy generation. The control loop for cooling the building also consists of a sensitive thermal storage unit and a thermal absorber surface for active cooling of the thermal storage tank. Inside the building, the room is heated by underfloor heating. The heat is extracted from the object of investigation via ceiling cooling. The usage of the room is assumed to be office like. The control loops are equipped with constant mass flow pumps.

The collector loop is controlled as a function of the total solar radiation (diffuse and direct radiation). If the total solar radiation on the south-facing vacuum tube collector (Coll_W_m^2 ; slope 45°) rises to over 100 W/m^2 , the pump P_C_W_MFLOW of the collector loop receives a signal and is switched on. Thus, the sensitive thermal storage tank heats up continuously. However, this control is only carried out until the temperature at the outlet of the collector exceeds the average temperature of the storage tank. This is to prevent the storage tank from losing heat via the collectors and being actively cooled down. However, the pump P_C_C_MFLOW of the absorber loop is only put into operation as soon as the irradiation on the absorber surface Coll_C_m^2 reaches 0 W/m^2 and the ambient temperature is below the average temperature of the cold sensitive thermal storage. This prevents the pump from heating up the storage tank on warm summer nights and allows heat to be radiated to the environment or horizon. The structural boundary conditions are based on a nearly zero-energy standard.

There are three main operating modes for the comfortable operation of the building: (1) the building is heated by underfloor heating, (2) heat is extracted from the building by ceiling cooling, (3) neither heating nor cooling of the building is necessary. The system is controlled in such a way that simultaneous heating and cooling operation via the pumps P_FH_MFLOW and P_CC_MFLOW is excluded. The regulation of the building is performed on the basis of the outside temperature. If the average outdoor temperature of the last 24 hours drops below 15°C , heating of the building is enabled. If, on the other hand, the outdoor temperature rises above 15°C , cooling of the building is enabled.

In order to identify the influence of the variation of individual parameters on the overall system, the object of investigation was equipped with state-of-the-art technical installations. Figure 2 shows the simulation results on the basis of the comfort band with a dimensioning of the system technology according to approved technical rules.

It is obvious that the system is not able to maintain indoor comfort at low outdoor temperatures. By enlarging the collector surface, a large part of the hours can be brought into the comfort band. Further investigations will determine the influence of the variation of climate conditions, variation of ventilation and of air-conditioning systems, and variation of usage.

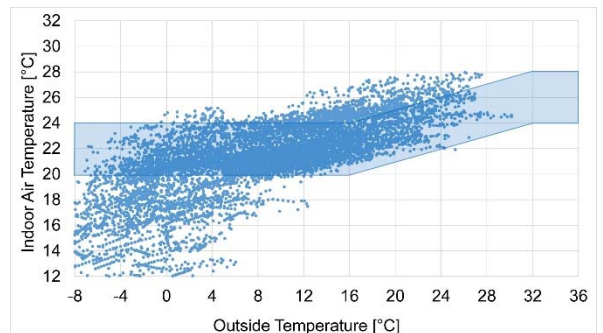


Figure 2: Results of system and building technology based on the comfort band according to DIN EN 15251

Additional revenues for biogas plants within Smart Market solutions in South Germany

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To fulfill international goals to reduce carbon dioxide emissions, the German government stated within the coalition agreement to further support the expansion of renewable energies and to evolve a share of 65% of gross electricity consumption by renewable energies by the year 2030. [1] Currently, the grid expansion and the increase of the renewable energy do not evolve synchronously and leads to loss of electricity production as part of the German congestion management. The energy throttled in 2017 amounts to 5.518 GWh – exceeding the highest amount so far. Related costs due to compensation payment to plant operators reached the number of 610 Mio. Euro in the year 2017. Most of the plants (84%) affected by congestion management actions are currently connected to the distribution grid. [2] To handle this situation in an effective way different steps are taken.

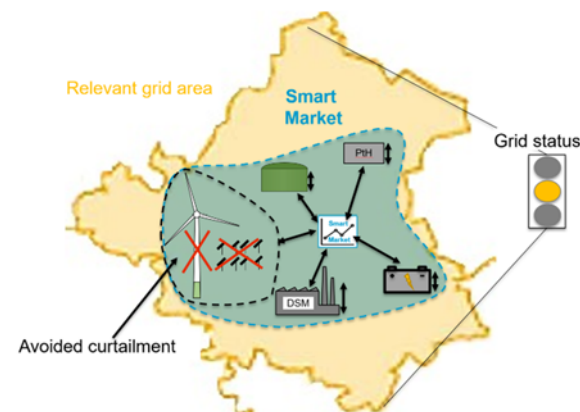


Figure 1: Competition of Smart Market participants during congestion period

On a medium-term point of view different approaches, which include the idea to bring market and grid together, can be one option to manage congestion situations in an effective way. To shorten the amount of curtailment and to help to reduce costs for compensation payment the establishment of Smart Markets during congestion time series are focused in the research. These markets are temporary and locally limited to grid areas and could be a supplement to the existing electricity and control power market in Germany. Participants within this market offer their flexibility to help to avoid the throttle of renewable energies.

In this work the role of flexible biogas plants within Smart Markets are focused. Among the renewable energies, flexible biogas plants can shift production easily to help to defuse the situation of congestion. The overall question is if biogas plants can help to not only reduce curtailment of photovoltaic and wind but also obtain further revenues within

a Smart Market. This additional revenue for flexible biogas plants could contribute to ensure profitability after the first EEG-period. Therefore the occurrence of Smart Market situations during congestion time series are analyzed to figure out in which regions of Germany and during which time periods this additional revenue could be attractive for biogas plants. Besides biogas plants other little generation units like natural gas plants and loads such as Power-to-Heat or battery storage are competing with each other. The individual cost structure for participants are estimated and general requirements for participating are analyzed. The goal is to help to implement sustainable solutions (focus biogas plants activities) during times of grid congestions without the curtailment of wind and photovoltaic.

References:

- [1] Koalitionsvertrag (2018): Koalitionsvertrag zwischen CDU, CSU und SPD, Ein neuer Aufbruch für Europa Eine neue Dynamik für Deutschland Ein neuer Zusammenhalt für unser Land, Berlin, den 12. März 2018, 71
- [2] Bundesnetzagentur (2019): Monitoringbericht 2018, Stand: 8. Februar 2019, 25-26, 144

Simulation-based identification of energy flexibility in a medium sized manufacturing company

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The expansion of renewable energies will have an increasingly negative impact on grid stability. Flexibilities in industrial production are one way of meeting this challenge. The prerequisite for this, however, is that these production flexibilities and the potential for targeted load shifting and reduction are known and evaluated both technically and economically. Knowledge of flexibility in production provides companies with additional competitive advantages through the marketing of flexibility in the energy trading market in addition to production-side advantages.

The aim of the ongoing research project is the systematic identification and evaluation of the flexibility of the production system and the optimization of the load profile while adhering to production key figures, such as throughput time and delivery reliability of the company Oswald in Miltenberg. Starting point of the model development is a detailed data collection of both production data and energy consumption. Based on this data, a model was created, that simulates the production process and is able to generate a synthetic load profile. The model can be used to determine the energy flexibility of the production system by varying switch-off intervals and the duration of switch-offs of production stages as well as by changing the production sequence. First, it is shown how flexibility with regard to energy demand and performance affects the delivery targets on the basis of the aforementioned production interventions. Figure 1 shows an example of the influence of changes in the production process on the resulting load profile.

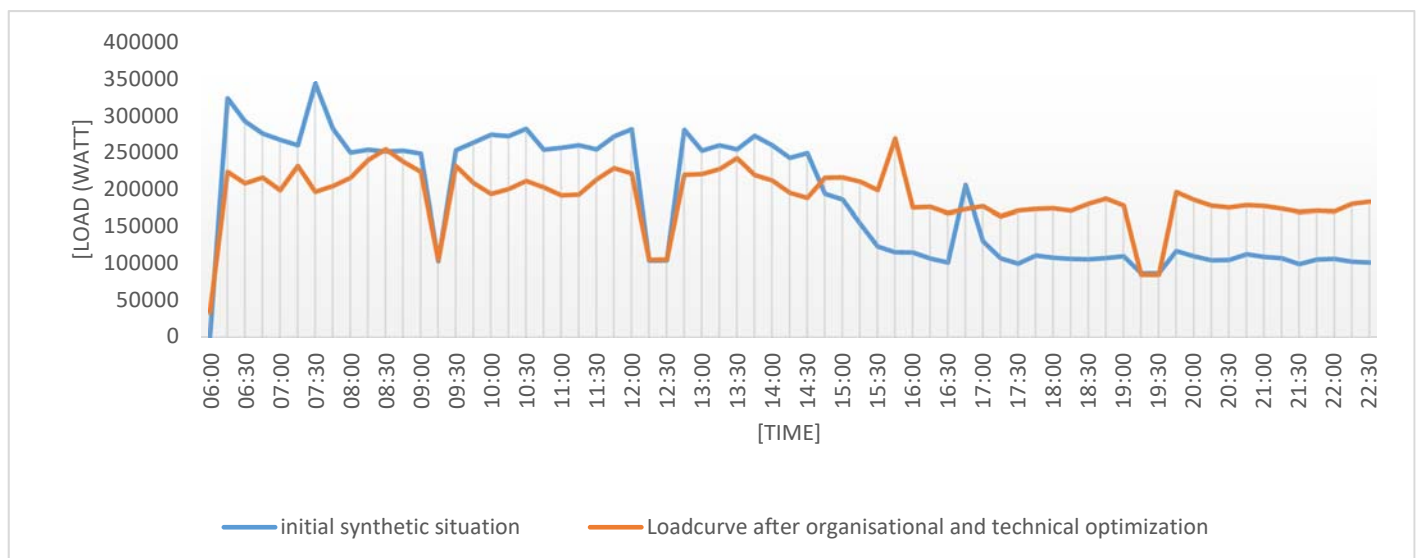


Figure 1: Result of the organizational and technical load profile optimization (daily load profile)

Literature (selection)

Eley, M. (2012). Simulation in der Logistik. Berlin Heidelberg: Springer Verlag.

Gahm, C., Denz, F., Dirr, M., & Tuma, A. (2016). Energy-efficient scheduling in manufacturing companies: A review and research framework. European Journal of Operational Research, S. 744-757.

Liu, Ying; Dong, Haibo; Lohse, Niels; Petrovic, Sanja; Gindy, Nabil (2014). An investigation into minimising total energy consumption and total weighted tardiness in job shops. Journal of Cleaner Production 65, S. 87–96. DOI: 10.1016/j.jclepro.2013.07.060.

Multi-Energy Management and Aggregation Platform

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In connection with the ongoing energy system transformation in Germany, great attention is being paid to the building sector with regard to unlocking efficiency potentials and integrating renewable energies. As a result, the building and energy sectors are becoming more interconnected to face interests and challenges from an integrated perspective. Buildings and their systems technology shall no longer only be passive heat and electricity consumers, but also be able to offer services to the energy system in form of flexible decentralised energy generation and storage capacities in connection with intelligent demand management. The progressive coupling of heat and electricity and interfaces to other sectors, such as mobility, makes this task even more complex. This forces a shift of the perspective away from individual buildings to building networks in the context of the overall energy system.

On the other hand the energy supply of existing buildings is mostly planned and operated isolated from their environment: If available at all, Energy Management Systems (EMS) do not work cooperatively and consider heat and electricity only separately. Local plants in the buildings are often old, inefficient or oversized.

The project **“Multi-Energy Management and Aggregation Platform (MEMAP)”** (FKZ 03ET1413B) addresses these challenges and develops and tests an open aggregation platform for the energy-efficient operation of buildings in a compound. The software platform coordinates independent energy management systems (EMS) to exploit synergy effects between different demand and production profiles.

Model predictive control methods are developed and integrated in the platform. This makes it possible to plan the optimal power and heat flows for a given building, infrastructure and equipment configuration within a prediction horizon. For the optimization different criteria (e.g. efficiency, CO₂ Emissions etc.) can be considered. A safe and reliable communication between the platform and the local EMSs is ensured by the use of OPC UA and BACnet as communication protocols.

Within the framework of the project, economic aspects will also be considered and possible business models for the use of the platform by various stakeholders will be drafted. From the functionality of the platform it is intended to derive a planning tool which is compatible with the BIM standard. Furthermore, the developed aggregation platform will be implemented, tested and evaluated under realistic conditions. This will take place in the CoSES microgrid laboratory at TUM. The emulated and investigated scenarios will be based on the situation in a small village near Munich and will be fed with measured data from there. Based on the test results, further analyses are carried out and the energy, ecological and economic potential and benefits are evaluated. From that recommendations for politics and industry are to be drafted.

The research project is carried out by TUM researchers in cooperation with six industrial and academic partners and is funded by the BMWi.

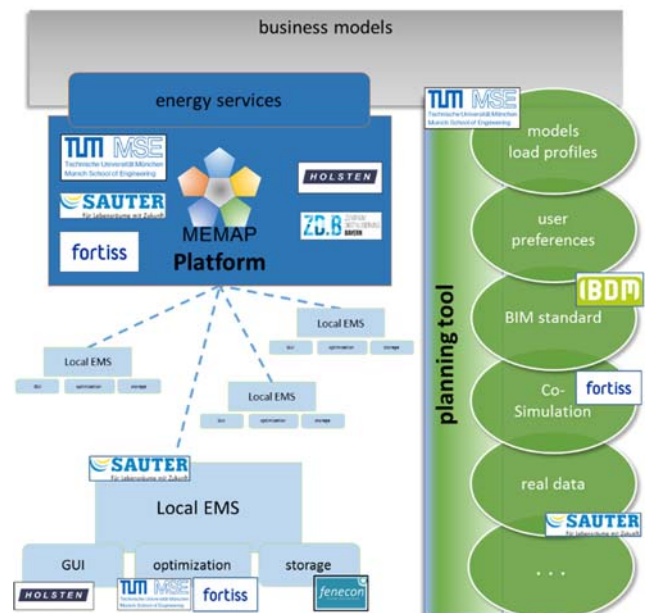


Figure 1: Idea, content and associated partners of the MEMAP-project



Smart Grid Technologies for Rural Areas and SMEs

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The aim of the Smart Grid project is to build up a cross-border laboratory of embedded systems between Bavaria and Czech Republic that fosters the integration of Small and Medium Enterprises (SMEs) into the Smart Grid and let them benefit from Smart Grid technologies. The University of South Bohemia in České Budějovice cooperates with the Technology Campus Freyung as project partner.

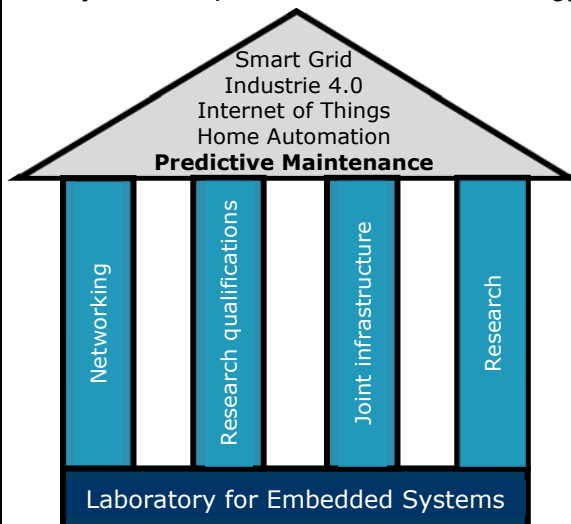


Figure 1: Smart Grid laboratory and research

Furthermore, smart grid infrastructure incorporates various intelligent devices to help optimizing both production and consumption ends. In the project we will focus mainly (but not exclusively) on the consumer's end. By implementing long-range remote consumption reporting (aka smart metering) together with optimization plans and security aspects of the data transmission from consumer back to the energy suppliers is possible to dynamically adjust actual power consumption of the consumer.

The main research goal of the laboratory will be to make current and future Smart Grid technologies available for small and medium enterprises (SMEs) and to integrate SMEs into the power planning process. These technologies represent mainly the smart metering, which allows to measure consumption on several levels (company, building, room, appliance), the automation of buildings (home automation) and the automation of production processes (Internet of Things, Industry 4.0).

In several case studies, regional small and medium-sized enterprises are surveyed about Demand Side Management. The goal of this is to find out which plants and processes are potentially suitable and how well the companies are familiar with this topic. SMEs will be enabled to benefit from researched technologies in terms of reducing their energy usage and in terms of reducing their energy cost. In the end, the savings lead to improving of the competitiveness of SMEs in the given region.

The combined volatility of both, power supply and power demand, creates a growing problem that needs to be solved by the Smart Grid. On one hand, volatile power demands lead to peak loads that need to be satisfied by inefficient peaking power plants, such as generators powered by fossil fuels. On the other hand, the increasing power production based on renewable sources tends to be subject to uncontrollable factors, e.g., wind or sunlight and power needs to be consumed as available. The Smart Grid needs to address this imbalance of power supply and demand and to maintain the power grid in a stable state. To achieve these goals, the Smart Grid realizes a complex energy management that tries to reshape power production and consumption and allows smooth integration of the regenerative energy sources.

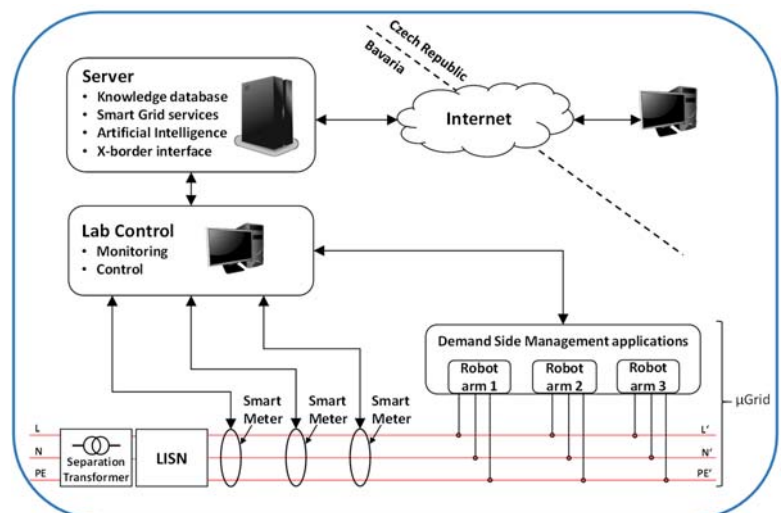


Figure 2: Planned laboratory infrastructure

Centre for Combined Smart Energy Systems – An introduction

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Smart grid research has reached a point of intersectionality where one specific field of research is inadequate to address the complexity of the problem at hand. The Center for Combined Smart Energy Systems (CoSES) is established as a part of Munich School of Engineering, which is an integrative research center in Technical University of Munich. CoSES covers fields of combined electrical and heat grid, power electronics, control theory, communication engineering and system integration to provide a holistic setup to test smart grid ideas.

Hardware-in-the-loop (HIL) philosophies are at the heart of the CoSES setup for both electrical and the heat grid with a communication grid for supervision (see Fig.1). The laboratory is designed as five individual houses (4 x Single family home + 1 x Multi-family apartment), which can be given any desired microgrid topology, and have access to the real electrical grid, PV modules, wind turbine emulator, electric car chargers and battery units. For the heat applications, each home has access to CHP, solar thermal emulator, power-to-heat, district heating and heat storage modules. Real life distances between these homes are implemented via a network of power cables (>1km) and heat modules which mimic the physical effect of transferring heat over a distance. A series of real-time processors and state of the art measurement modules shall provide online monitoring, high precision time series and variety of control choice for the grid operator.

Electrical loads are realized through bi-directional power electronic units operating as prosumers and a feedback grid. On-load tap changers and experimental inverter topologies are implemented to influence grid voltage control. Demand side flexibility through sector coupling is possible which could lead to less reliance on expensive battery storage systems. Three-temperature level heating grid allows for a low temperature district heating grid along with a possibility for district cooling system.

CoSES is thus positioned as an opportunity for research and industry partners to do among other things, benchmarking of smart grids, product development & functionality tests and evaluate smart grid operation strategies using a real grid setup.

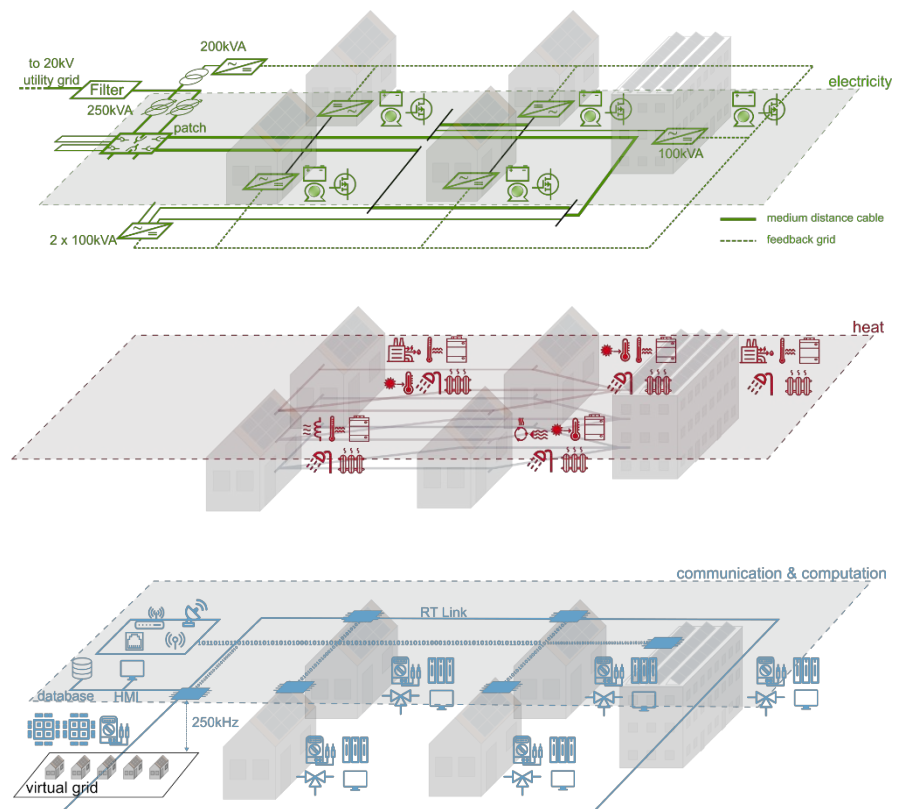


Figure 1: The 3-tier (electric, heat & comms) layer arrangement in CoSES

Impact of the Choice of Regions on Energy System Models

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Many existing energy system models rely on input data available at country-level, or at the level of administrative divisions. However, there is usually no correlation between the distribution of data such as solar radiation, wind speed, and electrical load on one hand, and the administrative divisions on the other hand. The goal of the research is to measure the impact of the shape of model regions on the results of system optimization models. A novel clustering methodology for high-resolution data is presented and applied to define new regions for an energy system model which optimizes expansion planning and unit commitment. The new model regions take into account the bottlenecks in the transmission system and their effect on the expansion of renewable energy sources. We compare the obtained energy mixes, new capacities, and curtailment levels against a model using administrative divisions. The results show discrepancies between the models in the case of a high share of variable renewable energy, and quantify the impact of the distribution of load, wind and solar resources on energy system models. Possible applications of the new model regions are discussed to emphasize their utility for modelers and policy-makers.

Development of rural communities in sub-Saharan Africa through decentralized Energy-Water-Food systems

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Limited purchase power in Sub-Saharan Africa impedes rural electrification by solar systems due to their high investment costs. Decentralized Energy-Water-Food systems have the potential to solve this problem. Using solar-powered water pumps, rural communities can increase their agricultural productivity. This enables profits by sales, so the initial investment costs of the solar system and water pumps can be paid back. Also, the increased amount of biomass waste enables economically feasible small-scale biomass digestion. The digestate serves as high concentrated organic fertilizer and the produced biogas can be used for electricity production by biogas motors in times of insufficient solar power generation.

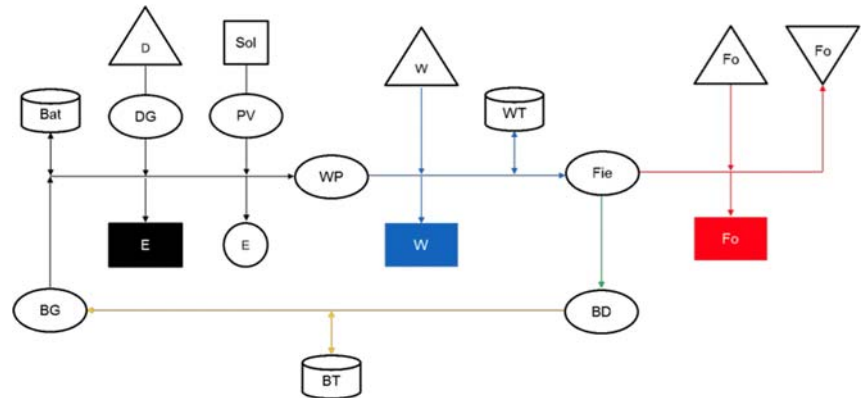


Figure 1: Scheme of Energy-Water-Food systems

In my research, these systems are analyzed in several ways: Data acquisition for site assessment by remote sensing, on-ground measurements and surveys, optimal system design by least-cost modelling including constraints such as ground-water potential to ensure sustainability; socio-economic requirements such as financing, entrepreneurial structures, sales potentials and training requirements.

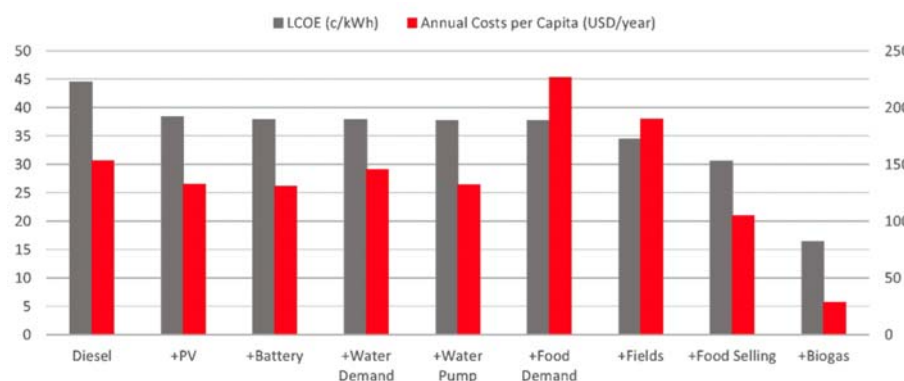


Figure 2: LCOE and annual costs per capita for each scenario

biogas production reduces the levelized costs of electricity (LCOE) from 0.45 USD/kWh by power supply from diesel generators to 0.16 USD/kWh. The modelling results shall support local governments and entrepreneurs in their decision-making.

To identify the least-cost system design regarding the supply of electricity, water and food for the rural village of St. Rupert Mayer, Zimbabwe, the linear optimization model *urbs* was adapted. *urbs* was developed for energy system model-ling, yet its sector coupling feature allows to add processes like water pumps and commodities such as biogas. The modelling results show that a holistic system including photovoltaics (PV), water pumps, enhanced agriculture and

Sewage sludge as a source of energy

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The treatment of wastewater and the resulting sewage sludge can be considered energy-intensive. Within the wastewater plant the aeration of the biological treatment stages and the water conveying technologies



Figure 1: Wastewater plant Mariánské Lázně (Chevak a.s.)

consume high amounts of electric energy. Furthermore the resulting sewage sludge requires additional treatment. In order to reduce its volume the sludge has to be dewatered. For this purpose high power centrifuges or chamber filter presses are used. In order to ameliorate combustibility and increase calorific value the sludge needs to be dried using thermal and electric energy (see Fig. 2). The incineration of sewage sludge can produce thermal or electric energy but needs additional fuel in order to achieve and maintain the legally required temperature. The thermal treatment often requires extensive transportation, since there is only a small number of centralised suitable facilities. The transportation of the sludge, often over long distances, additionally contributes to the cumulative energy balance. The energy efficiency of the treatment of

wastewater and the resulting sludge leaves room for improvement and it is of immense importance to define and to use these potentials.

For this purpose the German-Czech border region around Tirschenreuth on the German side and Cheb on the Czech side is selected for the analysis. The status quo of the waste water and sewage sludge treatment provides the reference scenario for potential ameliorations. For this purpose the existing disposal routes and procedures are assessed according to their energy consumption. In order to find a suitable procedure for sludge, the state of the art technologies available on the market are analyzed. The possibilities of co-fermentation of sewage sludge and other biomass in the wastewater plants equipped with a fermenter are identified in order to increase energy production from sewage gas. Further data is retrieved and analyzed in order to detect if sewage sludge drying with surplus heat from biogas plants is feasible. In order to address the energy demand of the transportation several calculated potential locations within the region are assessed and a program for the efficient transportation of sludge with optimized routes is designed. The focus is on the increase of resource efficiency and the decrease of greenhouse gas emissions. The aforementioned suggestions are combined into different scenarios, which are compared with each other for the evaluation. The evaluation is based on a Life Cycle Assessment. This analysis determines not only the energy consumption of the respective technology, but also the cumulative energy demand along the life cycle.

The main objective is an ecologically, technically and economically optimized process for the treatment of wastewater and sewage sludge in the sense of circular economy. Hence energy efficiency is increased, natural resources are preserved, greenhouse gas emissions are reduced and profitable value is created within the region.



Figure 2: Sludge drying facility in Neualbenreuth

Investigation of different treatment methods on semi-conducting polymer thin films to improve their thermoelectric properties

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Today, in times where problems like climate change, limitation of fossil resources and further increasing energy consumption are always present, the need for alternative solutions is clearly of immense importance for our future. So far, renewable energy sources like solar cells and wind power are of large interest and already commonly used. But people often forget to also think about ways to save energy and to reduce energy waste.

Nearly all processes in our daily life generate heat as byproduct, every engine, every electronic device, even the human body. This heat mostly just dissipates into the environment and cannot further be used. Including dissipating heat due to bad insulated buildings, in total roughly two third of our energy consumption is lost to the environment as so called waste heat.[1] Concerning that issue, we need techniques to reduce these significant amounts of wasted energy, to be able to overcome the world's energy problems in the future. Here, thermoelectric materials could be the solution, as they are able to convert a temperature gradient directly back into electrical power.

The underlying basic working principle for this conversion is the so called Seebeck effect. The Seebeck effect describes, that within a semiconductor (either p-type or n-type) an applied temperature gradient leads to a diffusion of the major charge carriers from the hot to the cold side. This diffusion creates an excess of major charge carriers at the cold and a lack at the hot side, resulting in an electrical voltage, called thermovoltage.[2]

So far, mainly inorganic thermoelectric semiconductors are commonly in use, as they provide good efficiencies.

However, they typically contain heavy elements, like bismuth, lead and tellurium, and are therefore rare, toxic, expensive and difficult to process.[3] Compared to that organic thermoelectric materials, for example conducting polymers are low or non toxic, they are lightweight, flexible and enable a low-cost solution based processability. Unfortunately, so far, the efficiencies for these polymer based thermoelectrics are low. In our research we investigate the thermoelectric properties of thin semi-conducting polymer films. By using different treatment methods, we attempt to affect the electronic and morphological features of the polymer and find ways to improve its thermoelectric properties. For investigation of the morphology-function relation, we use measurements of parameters such as Seebeck coefficient, electrical conductivity, absorbance, layer thickness and determination of the structure.

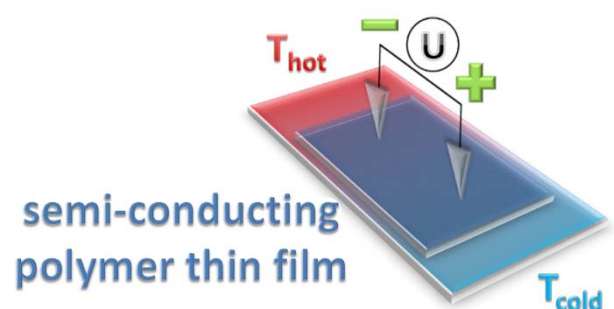


Figure 1: Thermoelectric principle

References

- [1] <https://www.sciencedaily.com/releases/2011/09/110920120238.htm>
- [2] O. Bubnova, X. Crispin, Energy Environ. Sci., 2012, 5, 9345
- [3] Q. Zhang, Y. Sun, W. Xu, D. Zhu, Adv. Mater. 2014

Techno-economic and Environmental Analysis of Utilization Pathways for Waste Sludge generated in a Paper Mill

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The utilization of waste streams is an inherent part of a sustainable development. Germany, the fourth-biggest producer of paper in the world, has a huge potential for an efficient treatment of waste sludge generated in paper mills. The produced sludge is declared as waste and the disposal can be costly. The goal of the project is to assess different utilization pathways by investigating them under techno-economic and environmental aspects. The technologies are evaluated for an exemplary paper mill.

There are three major types of sludge in a paper mill. The amount and composition of the generated sludge can differ depending on the used raw materials, on the produced products and on the technologies used in the paper mill. If waste paper is deinked, the process produces deinking sludge that contains short fibers, fillers and ink. During the preparation of the fiber suspension, the screening process separates unusable fibers and other rejects like plastic or sand that end up in the fiber residue. The third type of sludge is sewage sludge that is produced in the wastewater treatment plant.

Currently, the preferred option for disposing the sludge in the paper industry is the thermal treatment on-site or the disposal by third party services. The exemplary paper mill under investigation produces all three types of sludge and has no possibility to thermally use the sludge on-site. Therefore, other possible pathways are investigated to provide a cost efficient and environmentally friendly treatment of the generated sludge. New and innovative approaches are investigated and compared to the current utilization paths. From a variety of technologies, the most promising are analyzed in detail by calculating energy and mass balances. Examples for technologies are sludge drying by using waste heat or hydrothermal carbonization of sludge. Furthermore, the integration of the investigated concepts in the paper mill's energy system are checked. These concepts are evaluated according to their economic performance. In addition, an environmental assessment based on greenhouse gas emissions is performed. The analysis provides information about the best-suited system to increase the competitiveness of the paper mill and to simultaneously decrease the environmental impact. Results and conclusions can be transferred to other paper mills.

Optimization of Thermocline Heat Storage for Waste Heat Recovery with ORC

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It has been estimated that more than 300 TWh/y of waste heat is available from industrial processes in the European Union, whose largest part is found at 200-300 °C [1]. In this temperature range, Organic Rankine Cycle (ORC) power systems are among the most efficient technologies to convert the waste heat into electricity or combined heat and power. If the waste heat fluctuates over time, heat storage can be a viable solution to level off the fluctuations and guarantee better economic performance of the heat recovery system. The thermocline heat storage combines the classical hot and cold storage tanks in a single tank by means of an inner temperature gradient. It has the potential for high cost reduction by replacing expensive storage fluid with cheap filler material. For this reason, the techno-economic optimization of a thermocline heat storage combined with an ORC power system is here considered.

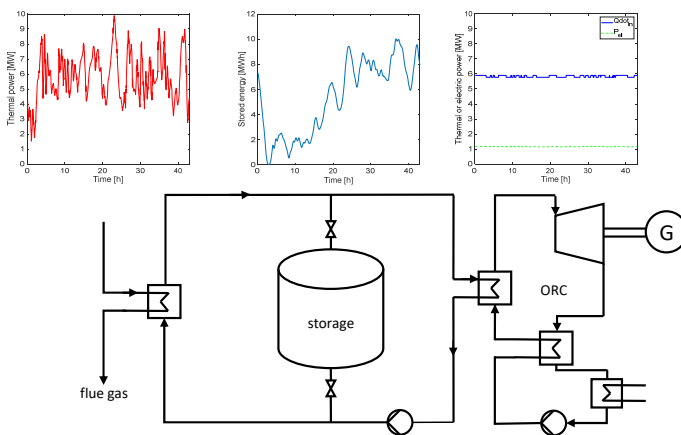


Figure 1: Waste heat recovery with thermocline tank and Organic Rankine Cycle power system.

The thermocline storage consists of a cylindrical tank with filling solid material (quartzite rock/sand). The heat carrier flows from top to bottom during charge of the storage and vice versa during discharge. The model is based on [2]. The thermocline storage is discretized as finite volumes along the height of the tank. The thermocline model has been validated against simulative and experimental data available in [2] and [3]. The results show a relative root mean squared error in temperature distribution of the solid material below 2 %. The ORC is estimated from the thermal power available from the storage. Its part-load and costs are determined from empirical correlations.

From the results, it is convenient to design the storage for the maximum energy required to level off completely the fluctuations, mainly because the ORC investment costs are much higher than the ones for the storage tank. The optimal tank has 4.8 m diameter, 14.4 height and 18.8 K cut-off temperature (Levelized Cost of Electricity, LCOE, at 3.5 ct/kWh). A sensitivity analysis is also carried out for different interest rates and considered periods of time. The LCOE increases almost proportionally with the interest rate. The LCOE would be higher than 9 ct/kWh for a period of only 5 years, and it would drop below 3 ct/kWh for 15 years and maximal tank size. Future work will consider a more detailed model of the high temperature heat exchanger between the heat source and the heat carrier as well as of the model of the ORC unit.

References

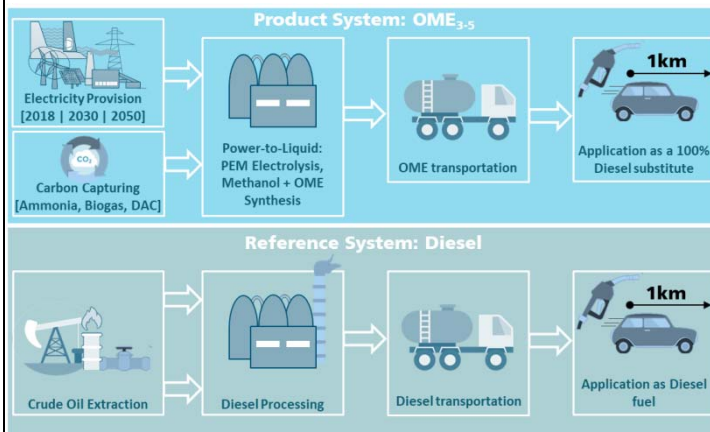
- [1] Papapetrou, M.; Kosmadakis, G.; Cipollina, A.; La Commare, U.; Micale, G. Industrial waste heat: Estimation of the technically available resource in the EU per industrial sector, temperature level and country. *Appl. Thermal Engineering*, vol. 138: pp. 207-216, 2018.
- [2] Modi, A.; Perez-Segarra, C. D. Thermocline thermal storage systems for concentrated solar power plants: One-dimensional numerical model and comparative analysis. *Solar Energy*, vol. 100: pp. 84-93, 2014.
- [3] Pacheco, J.E.; Showalter, S.K.; Kolb, W.J. Development of a Molten-Salt Thermocline Thermal Storage System for Parabolic Trough Plants. *Journal of Solar Engineering*, Vol. 124: pp. 153 – 160, 2002.

Life Cycle Assessment of Synthetic Fuel

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The study investigates whether the electricity based fuel "oxymethylene ether" (OME) can be an environmentally friendly alternative to diesel.



The analyzed OME production process is currently under development at the Fraunhofer Institute for Solar Energy Systems in Freiburg, Germany. The process is based on the synthesis of recycled carbon dioxide and renewable hydrogen. Synthetic energy carriers of this kind enable the transfer of renewable electricity into the mobility, industry and building sectors. Due to their suitability as chemical energy storage, these fuels may contribute to substituting the fossil raw material basis of these sectors and thus promote climate protection.

Figure 1: System Boundaries and Functional Unit

OME is systematically analyzed within the scope of a life cycle assessment (LCA) and compared with diesel. The work comprises a LCA model built with the help of UmbertoNTX and Ecoinvent, with underlying OME synthesis simulations performed in ChemCad and electricity generation simulations performed with Matlab. The analysis yields a quantitative understanding of environmental impacts caused during the production and use of both fuels. In this context, special attention is given to the carbon balances and the resulting global warming potentials. Several forecasting scenarios evaluate Germany, Norway and Morocco as potential locations for OME production until 2050. The assessed sources of carbon dioxide include ammonia production, biogas upgrading and the capturing of CO₂ from ambient air.



Figure 2: Fraunhofer ISE building in Freiburg

The following key messages can be derived:

While in the case of diesel, most environmental impacts occur in the form of exhaust pipe emissions, the operation of electrolysis is the decisive parameter within the OME life cycle. Provided that OME production is partly supplied with grid electricity in Germany or Morocco, its life cycle emissions are very likely to significantly exceed those of diesel. This conclusion applies to any source of CO₂ and is considered to stay valid in the mid-term (2030), notwithstanding the ongoing defossilization of the background electricity systems. On the other hand, the Norway scenario revealed that the evaluated synthesis path is generally suitable to produce OME with a favorable global warming footprint. It is important to consider though that an overall slowdown of the atmospheric greenhouse gas accumulation can only be achieved, if the recycling of CO₂ leads to a substitution of fossil resources at least by the same amount.

E2Fuels - Assessing the role of Renewable Low-Emission Fuels in Tomorrows Energy System and Mobility Sector

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While Germany's target of 35 % renewable energies in the electricity sector by 2020 could already be achieved ahead of schedule, the share of renewable energies in the transport sector is declining (5.2 % in 2015). For this reason, significant efforts and new approaches are needed to increase the share of renewable energies and reduce greenhouse gas emissions in the transport sector. A promising way to achieve these goals is the use of synthetic fuels. These are synthesized with hydrogen from electrolysis and additionally incorporate carbon dioxide. Hence, they offer the opportunity to use the increasing share of renewable energies in the electricity sector and the learning curve effects in photovoltaic and wind energy plants in the transport sector. At the same time they could contribute to the flexibilisation and integration of fluctuating renewable energies in the electricity sector.

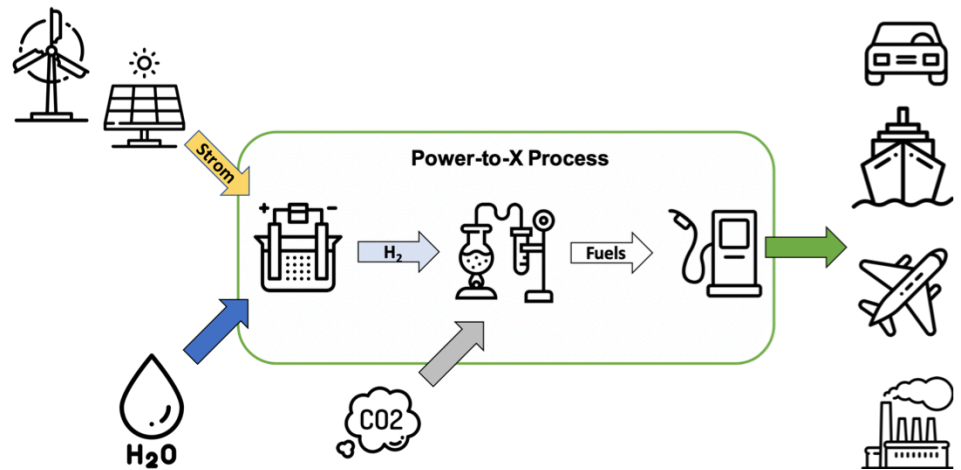


Figure 1: Overview of Power-to-X processes

In the E2Fuels project the Chair of Energy Systems is investigating the production and use of synthetic fuels.

For this purpose, the entire path from surplus electricity to the platform chemicals hydrogen, methane and methanol is thermochemically modelled. The project focuses on electrolysis and various synthesis routes. In order to achieve maximum efficiency, perfect integration of heat and by-products is essential. With the aid of an optimization algorithm, the size of the buffer storage tanks and the size of the plant components is optimized. In system simulation of the German and European energy system, interactions and synergy effects on other sectors are evaluated. This holistic approach promises a sustainable design of the production of E-Fuels.

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e²Fuels
Erneuerbare Emissionsarme Kraftstoffe

Sector coupled Smart Energy Management System for operational flexibility in a real Microgrid

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In modern microgrids, operational flexibility is crucial to prevent high investment costs for oversized energy buffers. In the Center for Combined Smart Energy Systems (CoSES), which is part of Munich School of Engineering, a real microgrid is being build up. To ensure operational flexibility and an optimal distribution of a microgrid's resources, a smart Energy Management System (EMS) is needed. Different EMS's have already been designed in literature. Some of them cover the electricity grid but do not take into account the heat grid. Other works include heat storage components but do not provide experimental evidence of the system operation.

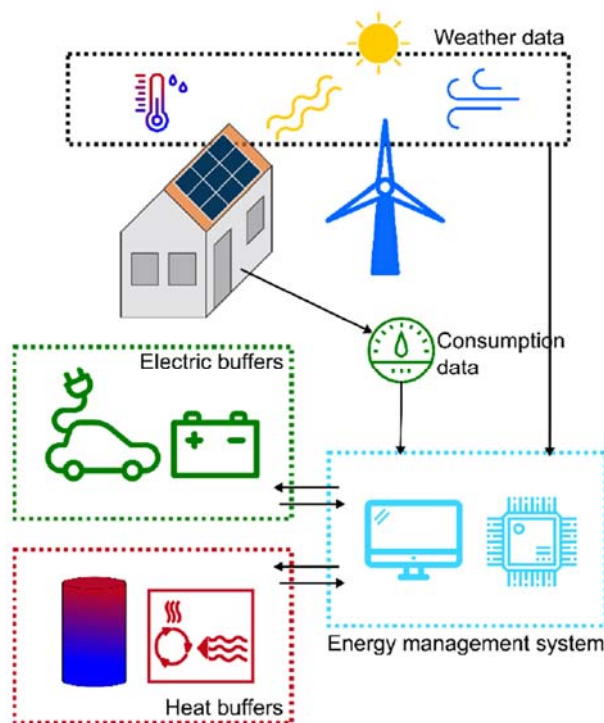


Figure 1: EMS idea for two kinds of energy buffer

In this work, a smart EMS model will be simulated using MATLAB and Simulink to optimize energy transactions between generation and consumption units to provide maximum economic advantage to the consumer and reduce the overall energy consumption of the microgrid. Furthermore, the environmental impact should be reduced by using renewable energy production and intelligent storage techniques. The EMS should then leverage the sector coupled energy resources to provide load-shifting options to reduce the dimensioning of energy storages.

The CoSES laboratory provides electrical energy buffers, such as electric car charging stations and a stationary battery as well as heat buffers, consisting of a heat pump and several heat storages. The microgrid's household loads will be simulated by CoSES with bi-directional converters. The energy production will be mostly covered by a 20kW photovoltaic power plant to provide the microgrid with renewable energy. By means of a modern weather station the household load and the PV generation forecast data will be adapted to generate real-time circumstances. After implementing the model in CoSES microgrid, experiments will be run to either validate the test cases or iterate for better results.

Sunny islands – a danger to the grid?

Investigation of economic environment leading to grid independent operation of industrial sites

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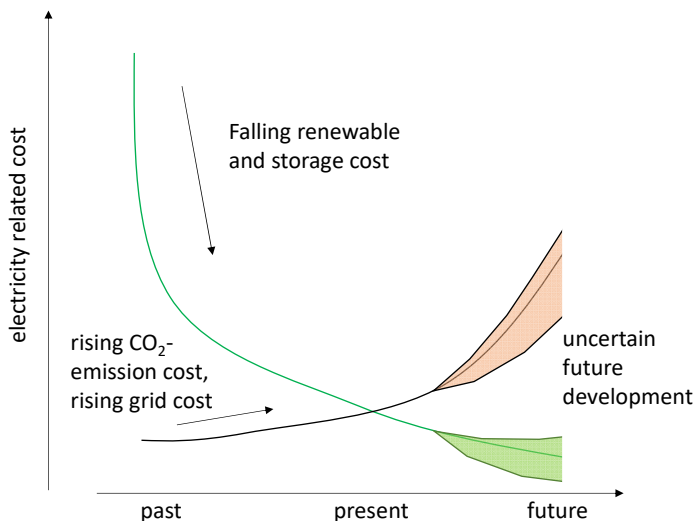


Figure 1: Evolving boundary conditions for electricity cost and future uncertainties

Macro trends and local developments are currently shaping the future of our energy system. Developments such as local and national attempts, supported by international agreements, to become mostly carbon neutral within the next decades, result in uncertainties for industries regarding future commodity and CO₂ emission cost. Falling costs for renewable electricity generation and storage options are occurring, while at the same time grid related costs, taxes and fees make up more than 70% of typical industry electricity cost. If local PV for self-consumption is installed, the lower resulting consumption from the grid can lead to even higher specific cost of grid-supplied electricity.

The research question investigated in this work is under which conditions regarding renewable technology cost, grid-cost, CO₂- and gas price, as well as storage cost development, islanding will be cheaper for industries than being connected to the grid. Grid connection includes either purchasing all the electricity or producing a part of the electricity onsite by renewable or conventional means. The investigations are performed via a combination of cost equations based on literature research for conventional technologies (namely gas engines and gas turbines) and linear optimization to determine the optimal storage to renewable generation ratio depending on load profiles and renewable generation time series.

The results allow companies facing investment decisions now to take into account possible future developments and enable politicians to shape laws and regulations in such a way, that unnecessary macro-economic costs (e.g. oversized grid because supplied companies decide to change to island mode) may be avoided.

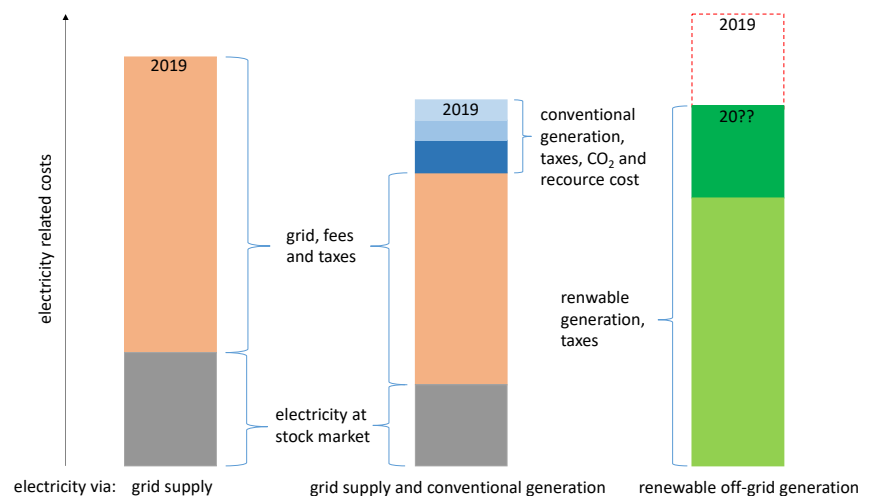


Figure 2: Schematic cost structure of different possible electricity generation modes

Combined Heat and Power Generation by Enhanced Geothermal Systems

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The utilization of hydrothermal resources for combined heat and power generation is an attractive alternative for providing renewable electricity and heat, as it can be seen exemplary by the increasing numbers of installed projects within the South German Molasse Basin. However, such favorable geological conditions as it is the case for the southern parts of Bavaria are not common. Therefore, while the utilization of hydrothermal resources is limited to certain geological regions, Enhanced Geothermal Systems (EGS) have a tremendous technical potential without major regional restrictions. In the last years, an increasing focus is laid on the utilization of EGS with supercritical CO₂ (sCO₂) instead of water due to its beneficial fluid characteristics.

Existing studies present several different concepts for power generation from sCO₂ EGS. Next to the direct expansion of the sCO₂ in a turbine, also the application of the sCO₂ solely as heat carrier for an Organic Rankine Cycle (ORC) system as well as the combination of a direct expansion and an ORC system is investigated. Concerning the utilization of EGS by water, several potential plant layouts are discussed. Direct expansion by single or double flash plants as well as their combination with an additional ORC as binary cycle are possible. Depending on the achievable temperature level of the brine and as well avoiding potential corrosion issues within the components in case of direct utilization, also the sole application of an ORC as a binary power plant may be advantageous.

However, the current development of the geothermal sector in Central Europe increasingly emphasizes the combined heat and power generation (CHP). Consequently, the annual available heat flow for power generation could vary strongly due to the changing heat demand. Thus, an assessment of the potential different power plant types for EGS should consider the part load characteristic of the plant layout, instead of assuming constant full load operation.

Based on the heat demand characteristic of an actual district heating network, this study investigates the performance of the above-ground plant, comparing sCO₂ and water as heat carrier for the utilization of the EGS. The performance of both options is evaluated with respect to different temperatures of the geothermal reservoir. The results present a recommendation regarding the most suitable plant layout and heat carrier medium for EGS projects in case of CHP operation. The work provides a valuable contribution to the debate about suitable plant concepts for EGS projects against the background of combined heat and power generation.

Crowd size estimate with thermal imaging

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Crowd-centric research is receiving increasing attention as greater amounts of data sets become available allowing to capture various behavioral aspects of big groups of people. Nevertheless, achieving high accuracy while keeping a low energy consumption and preserving the privacy of the involved subjects is of great challenge.



Figure 1: Segmented thermal image

In this work, we address the problem of crowd size estimate by employing machine learning for object detection in thermal images, exemplified by Figure 1. One of the main advantages of this technique is the privacy preserving aspect of these infra-red images. When compared to their RGB counterpart, infra-red frames contain little personal information such as facial features of those being recorded.

Such systems could be deployed in crowded areas where an accurate real-time estimate of head-counts is needed over a long period of time. This would allow long term assessments of which areas attract more people, how a big crowd is formed and how long it takes for it to disperse in big public spaces.

Furthermore, scientific experiments where accurate estimation of crowd sizes is needed could use this head-count as its ground truth.

Alternative methods include: (a) the use of trained personnel, which may be costly and not easily scalable; (b) wireless passive measurements which often assume members of the crowd to be carrying some mobile device, such as smartphones or RFID/Bluetooth tags, and may store temporarily a unique identifier of these devices raising privacy concerns; or (c) proximity sensors which often have limited coverage.

Using state-of-the-art image segmentation techniques our system (exemplified in Figure 2) aims at accurately estimating crowd sizes in public spaces while using constrained devices, such as Raspberry Pi's. In this way, we develop a portable and easy to deploy crowd estimate system. Furthermore, captured frames can be stored for offline processing to improve existing models while preserving the privacy of the subjects involved.

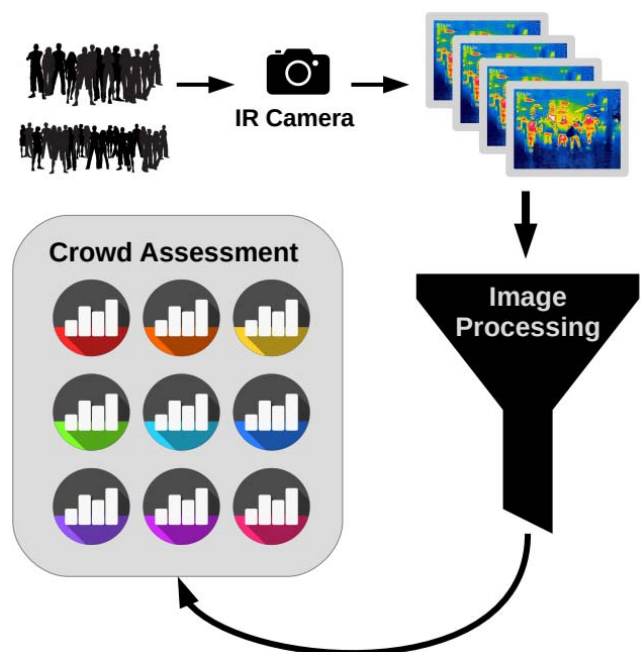


Figure 2: System design, exemplifying the pipeline of assessing different properties of a crowd using thermal images.

Influence of Cathode Ionomer Content on Hydrogen Permeation Rate in a High Pressure PEM-Electrolyzer

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PEM water electrolysis is one of the most promising technologies for CO₂-neutral future energy scenarios.

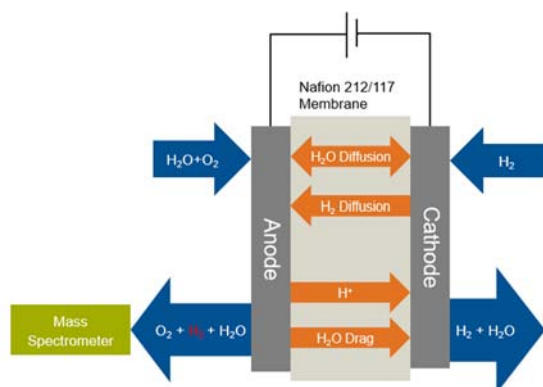


Figure 1: Setup for in operando hydrogen permeation rate measurement with a mass spectrometer

Electricity from renewable sources can be used to produce hydrogen for large scale energy storages and mobile applications. In order to increase the efficiency of a PEM electrolyzer, especially at high current densities, thinner membranes than the state-of-the-art Nafion® 117 can be used to reduce ohmic losses. However, thinner membranes exhibit higher gas permeation resulting in a decreased faradaic efficiency and safety issues. In this study, the hydrogen crossover in a PEM electrolyzer cell (1) is measured with a mass spectrometer during operation at current densities of 0-6 A/cm² and pressures of 1-30 bar (differential). Membrane electrode assemblies (MEA) with iridium as oxygen evolution catalyst and carbon-supported platinum as hydrogen evolution catalyst on Nafion® 117 and Nafion® 212 membranes are analyzed and compared. The influence of high ionomer content in the cathode electrode was investigated in particular.

A strong current dependence of the hydrogen permeation rate through the membrane is observed for cathode ionomer to carbon weight ratios higher than 0.6, which is most pronounced at low pressures and current densities higher than 2 A/cm². The results are compared to other studies (2, 3), that partially observed similar effects for current densities lower than 2 A/cm².

One possible explanation for the significant current dependence of the hydrogen crossover are mass transport limitations in the cathode, leading to a local pressure increase, which results in an enhanced hydrogen diffusion rate. By increasing the ionomer content in the cathode catalyst layer, this local increase in pressure is even more severe. The influence of this effect is investigated and discussed in this study.

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References:

1. M. Bernt and H. A. Gasteiger, *Journal of The Electrochemical Society*, **163**, F3179 (2016).
2. P. Trinke, B. Bensmann and R. Hanke-Rauschenbach, *International Journal of Hydrogen Energy*, **42**, 14355 (2017).
3. M. Schalenbach, M. Carmo, D. Fritz, J. Mergel and D. Stolten, *International Journal of Hydrogen Energy*, **38**, 14921-14933 (2013).

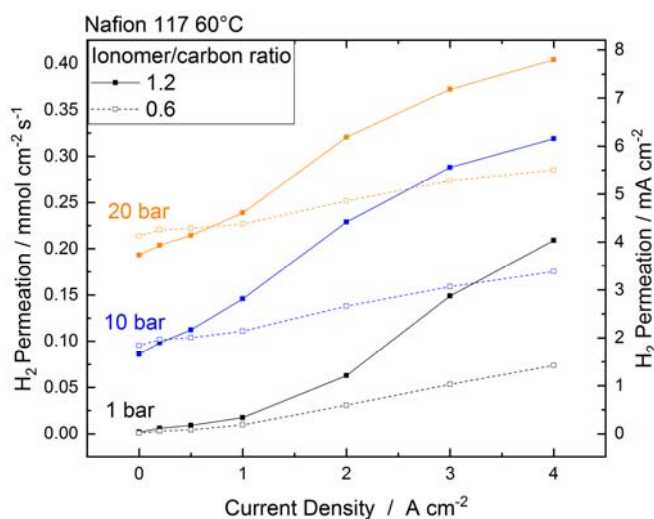


Figure 2: Hydrogen permeation rates for MEAs with a Nafion® 117 membrane at 60°C and hydrogen pressures of 1-20 bar (oxygen anode at ambient pressure), curves for ionomer/carbon ratios of 0.6 and 1.2