Munich School of Engineering
Technische Universität München

New Concepts in Energy Science and Engineering

6th Colloquium of the Munich School of Engineering

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The advances in shaping the Munich School of Engineering (MSE) are recently easily observable through the progress in the formation of our new building for energy and information (Zentrum für Energie und Information) which will host the MSE in future. Three energy laboratories will enable research in organic PV cells, new batteries and micro-grids. The micro-grid laboratory, CoSES (Combined Smart Energy Systems Research Laboratory), will be capable of emulating from current passive distribution grids up to future smart-grids. The transformation of the distribution grid is one of the major challenges in the coming years and is strongly connected to the overall digitization initiatives. The optimal operation of these grids will require optimal use of modern communication and information technologies.
With the Geothermal Alliance Bavaria (GAB) a new research alliance within the field of geothermal heat and power was initiated. The project coordination between internal and external partners will be done within the MSE. Geothermal energy has the potential to play a major role in Bavaria and the Alliance is a brilliant opportunity to turn the potentials into reality.

Energy was again very high on the agenda in the last years, actually this time with lower oil prices than expected. Unfortunately, the price reduction did not boost the world economy as it did in the past. Still many aspects of the energy system are not yet well understood. This just emphasizes, research is necessary so that we have in future a better understanding of this very complex interplay between politics, society and technology.

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:

- 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.

The **Study Program Division** of the MSE provides currently one undergraduate and two graduate programs with emphasis on an interdisciplinary education in the field of engineering sciences. Talents in mathematics, natural science, and medicine get the chance to have a deep look on both, fundamental research in engineering and science as well as entrepreneurial viability of new technologies. This combination opens great professional opportunities in the interdisciplinary business fields of the future for MSE-graduates.

In **Engineering Science** (Bachelor of Science) students get a broad methodological and scientific training with a focus on mathematics and science subjects. In the fifth and sixth semester the concept of this program allows students to individually create their personalized specialization within engineering.

The **Industrial Biotechnology** program (Master of Science) qualifies science or engineering graduates in the field of white biotechnology. The four semester curriculum contains subjects of a wide spectrum regarding life science as well as process engineering, chemistry, physics, agronomy, robotics and information technology.

The program **Human Factors Engineering** (Master of Science) enables graduates to design and evaluate human-machine-interfaces in different technical domains. They can enhance the anthropometric design of workplaces from industrial production to aviation cockpits. Students are skilled to succeed in academic or industrial research, production engineering, safety management, or counselling.

The orientation program **studium MINT**, launched in summer semester 2014, aims towards High School Graduates interested in MINT (STEM) disciplines. Students are provided with a solid basis in the fields of Science, Technology, Engineering and Mathematics, before enrolling in a specific study program. After completion of the studium MINT, the graduates are better prepared to make an informed decision about their academic future.

Center for Power Generation

The Center for Power Generation (CPG) is a research cooperation established within the MSE involving multiple TUM institutes dealing with research on energy conversion. The CPG covers the whole spectrum of energy research, from the efficient generation to the intelligent distribution of electrical power. Thermal power plants still represent the backbone of the energy system. In order to accomplish the decarbonization of the energy sector, fossil fuels have to be replaced with renewable alternatives, such as biomass or geothermal heat. Furthermore, an increase of the power plant flexibility, an integration of energy storage and an adaption of the transmission network is necessary to ensure a reliable electricity supply in the future. Currently, three research projects are ongoing which demonstrate the interdisciplinary research approach of the CPG:

Nine researchers are involved in the project “Energy Valley Bavaria - Flexible Power Plants”. Experimental investigations of gas turbine combustion and steam generation are combined with theoretical approaches of power plant simulation and power system optimization.

In the “CleanTechCampus” Initiative, an interdisciplinary team of electrical, mechanical, civil and building technology engineers will develop an innovative energy master plan for the TUM Campus Garching as an example for highly integrated and decentralized city and industrial districts. Within the framework of the project, a methodology will be developed to simultaneously optimize electricity, heating and cooling supply and distribution, allowing exploiting synergies between the different energy sectors and identify key conversion technologies. This project is carried out in cooperation with the Center for Sustainable Building.

Within the newly founded “Geothermie-Allianz Bayern”, the CPG covers the research on power generation from geothermal heat. The subprojects “efficient and flexible power plants” as well as “monitoring” try to increase performance and reliability of geothermal power plants. Especially in the surrounding area of Munich, renewable energy from geothermal power station has a significant potential.

The CPG provides an innovative environment enabling efficient collaboration across faculty borders through the exchange of knowledge and resources from several institutes of the TUM. Furthermore, the CPG serves as a qualified contact for interested parties and potential partners, supporting the transfer and sharing of expert knowledge. To date 17 partners from four faculties share their expertise in the framework of CPG. New members are always welcome.

Network for Renewable Energy

The Network for Renewable Energy (NRG) is an interdisciplinary research network in the framework of TUM.energy within the Munich School of Engineering (MSE). NRG acts as a platform for TUM researchers working on renewable energy projects independent of their discipline.

The network is headed by Professor P. Müller-Buschbaum, Chair for Functional Materials, and was founded to create the opportunity to stem interdisciplinary, large-scale research projects but also to foster an active communication between different research groups.

The project TUM.solar is one of 5 key labs of the “Solar Technologies go Hybrid” program of the Bavarian State Ministry. Research is carried out within the TUM groups investigating hybrid systems of nanomaterials for more efficient use of solar energy and photo-catalysis. In regular scientific meetings exchange with the other four Bavarian universities is fostered.

The researchers forming the Network for Renewable Energy are from various departments from the TUM and associated institutes: the Bavarian Center for Applied Energy Research (ZAE Bayern), Centre of Life and Food Sciences Weihenstephan, Chemistry, Electrical Engineering, Informatics, Mechanical Engineering, the Munich School of Engineering, Physics, as well as the Walter-Schottky-Institut. Doctoral students within the NRG use the network to find collaborators and exchange know-how and facilities. Furthermore the network coordinates visits to laboratories and aids with finding research collaborators throughout the network.

Participation in the NRG is open for all TUM researchers interested in renewable energy conversion and storage and only requires an informal email to the organizers which can be found on www.nrg.mse.tum.de.

Science Center for Electromobility

The Science Center for Electromobility (Wissenschaftszentrum Elektromobilität – WZE) is a research cluster of multiple institutions from six different faculties at TUM working together on further progress in the field of electromobility. A wide spectrum of research is covered ranging from fundamental research on future battery technologies to applied science developing innovative vehicle concepts as well as vehicle-to-grid applications.

Based on the successful completion of the MUTE project in which an electric vehicle was developed and a prototype was built, further research regarding lightweight design, efficiency and safety of such an innovative type of vehicle could be accomplished within the Visio.M project. At the same time, TUM CREATE, the joint research program between TUM and Nanyang Technological University (NTU) in Singapore, finished its concept of an electric taxi and presented its prototype at the Tokyo Motor Show. The results of TUM’s activities in the field of electric vehicles are highly recognized on an international level.

Despite the fact that an increasing number of electric vehicles is being commercialized by car manufacturers, there remains a large number of research questions especially regarding their integration into the larger energy system. Hence, the Science Center for Electromobility as a member of the Munich School of Engineering can address these challenges with interdisciplinary research approaches which form a vital element of TUM’s energy activities.

Center for Sustainable Building

The main focus of the Center for Sustainable Building (ZNB) is to develop comprehensive solutions for the complex interdisciplinary challenges in the fields of sustainable and energy efficient building.

As a joint cooperation between the TUM chairs of Building Physics, Building Technology and Climate Responsive Design, Energy Efficient and Sustainable Design and Building as well as Renewable and Sustainable Energy Systems, the Center for Sustainable Building provides the basis for an extensive scientific exchange between various faculties – particularly the faculties of Architecture, Civil-, Geo- and Environmental Engineering, Electrical Engineering and Information Technology as well as the related centers of the Munich School of Engineering.

Due to the cross faculty composition of the Center, the expertise reaches from sustainable urban development and building design to the development of energy efficient façade elements and systems related to innovative solutions in the field of building services. The activities range from fundamental research to practical application and teaching.

With this interdisciplinary background, the Center is able to develop innovative solutions for the global challenge of climate change, as the building sector is holding an enormous potential for energy savings and the reduction of CO_2 emissions. In addition to this focus, the Center has recently initiated the Life-Cycle-Balance and Sustainability Lab to combine its research activities with advanced teaching methods and contents.

Center for Combined Smart Energy Systems

The transition from fossil to renewable energy systems raises scientific, technical and organizational challenges. A new regulatory framework needs to be found, which creates the necessary incentives for the construction of the new infrastructure. The coupling of different energy sectors (electricity, heat and transport) is a promising engineering solution.

The conversion of the conventional distribution grid to an active microgrid is an important prerequisite. The microgrid handles completely new control and management tasks, such as frequency and voltage control or the optimal coordination of distributed generation units, batteries and flexible loads. To increase the flexibility of the system flexible district heating grids can be added as an additional option.

The development of smart microgrids is imperative for tomorrows electric power system and for the success of the energy transition („Energiewende“) from a technical and organizational perspective. The Center for Combined Smart Energy Systems (CoSES) was founded at the MSE to develop scientific and engineering solutions for a future microgrid. The Center is an interdisciplinary platform, combining TUM‘s expertise in energy, control and communication engineering. The Center is open for scientific and industrial cooperation in the field of computer sciences, electrical and mechanical engineering to overcome the challenges of a grid fueled by various distributed and renewable energy sources, interconnected by a modern communication network.

Programme

8.30 - 9.00 am
Registration

9.00 - 9.15 am
Opening
Thomas Hamacher, Director Munich School of Engineering

9.15 - 9.45 am
Keynote: „How to Leverage Corporate Research to Lower the Cost of Wind Energy”
Dominic von Terzi, Manager Aerodynamics & Acoustics
GE Global Research

9.45 - 11 .00 am
Session Chair: Werner Lang, ZNB MSE

Demand Side Management Potential of Buildings in Germany’s Future Energy System
Florian Sänger, Institute for Energy Economy and Application Technology

Optimizing the Refurbishment of a Single Family Home
Johannes Maderspacher, Centre for Urban Ecology and Climate Adaption

Energy Management and Electromobility in Plus Energy Homes and Districts
Claudia Hemmerle, Centre for Sustainable Building

11.00 - 11.45 am
Poster Presentation, Coffee Break

11.45 - 1.00 pm
Session Chair: Peter Müller-Buschbaum, NRG MSE

Metal Electrodes in Organic Photovoltaics - Why Contact Matters
Franziska Löhrer, Chair for Functional Materials

X-Rays, Neutrons, and Positrons: Strong Contributors in Revealing Fundamental Processes in Lithium-Ion Batteries
Irmgard Buchberger, Chair of Technical Electrochemistry

Elucidation of Adsorption Processes at the Surface of Pt(331) Model Electrocatalysts in Acidic Aqueous Media
Daniel Scieszka, Research Group Physics of Energy Conversion and Storage

1.00 - 2.30 pm
Poster Presentation, Lunch Break

2.30 - 2.50 pm
Teaching at MSE
Andreas Kremling, Specialty Division for Systems Biotechnology

2.50 - 4.05 pm
Session Chair: Markus Lienkamp, WZE MSE

Large-Scale Power System Design - Improving Decomposition Techniques
Paul Stursberg, Chair of Applied Geometry and Discrete Mathematics

Towards Fuel Production from Biomass via Electrocatalysis and Catalytic Hydrogenation at Ambient Conditions
Oliver Gutiérrez, Chair of Technical Electrochemistry II

Optimal Feedforward Control of Permanent-Magnet Synchronous Machines in Renewable Energy Systems
Lorenz Horlbeck, Chair of Automotive Technology

4.05 - 4.50 pm
Poster Presentation, Coffee Break

4.50 - 6.05 pm
Session Chair: Hartmut Spliethoff, CPG MSE

OpenGridMap: Automatic Power Grid Simulation Model Generation from Crowdsourced Data
Jose Rivera, Chair for Application and Middleware Systems

Flexible Power Generation with Thermal Power Plants: Process Analysis Using Dynamic Simulation
Steffen Kahlert, Institute for Energy Systems

Wind Farm Control for Power Maximization
Johannes Schreiber, Wind Energy Institute

6.05 - 6.35 pm
Keynote: „Beyond Oil and Gas – Mobility of the Future“
Ferdi Schüth, Director at the MPI für Kohlenforschung,
Vice President of the Max-Planck-Society

6.35 - 6.50 pm
Summary of the Day

6.50 - 9.00 pm
Poster and Presentation Award, Colloquium Dinner

Contents

1 Oral presentations

Demand Side Management potential of buildings in Germany’s future energy system

Florian Sänger[a], Dennis Atabay[b], Manuel De Borja Torrejón[c], Rita Dornmair[d], Johannes Maderspacher[e]

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The German “Energiewende” with an increasing share of renewable power generation, especially from wind and solar energy, challenges the power system with its temporal fluctuations and geographical dispersion. Solutions to those challenges may be extensions of the electricity grid and storages but also sector coupling of the electricity system with the heating system (power to heat). Buildings, former passive consumers, can be turned into Demand Side Management (DSM) devices. Electric heating systems like heat pumps, controlled by advanced energy management systems can turn them into flexible loads. Several studies already show that using buildings as DSM devices can benefit the future power system.

In this joint research project three institutes of the Technical University of Munich investigate benefits of DSM in buildings using a model buildup, which couples detailed building models with an energy system optimization. The German building stock is represented by multiple building models. Each of these models can be supplied with different heating systems. DSM is implemented in buildings with electric heating systems using Model Predictive Control (MPC). It generates new electric load profiles for each building based on the price curve. Subsequently the energy system optimization generates a new price curve. The investigated period stretches from 2015 to 2050.

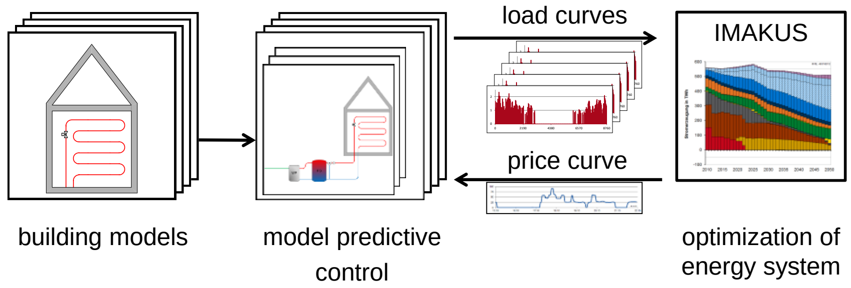

Figure 1: Modeling approach, coupling detailed building models with energy system optimization

The German building stock is represented by detailed building models. These models are structured by building types and age. This approach allows scaling the heat demand of each building model according to the represented share of building space. During the investigated period, refurbishments and new building types change the building stock.

Each building model can be equipped with conventional heating systems like gas and oil boilers as well as innovative systems like heat pumps or direct electric heater. To shift the electricity demand for heating, a model predictive control system is used. This approach generates cost optimized heating profiles based on time-sensitive electricity price curves. The main constraint for the MPC is maintaining the thermal comfort zone, which is ensured by using a penalty function. The generated load profiles are passed to the energy system optimization model.

Subsequently this optimization model calculates the influence of the new load profiles. The energy system model optimizes economic installation of power plants and their dispatch besides regarding large scale storage technologies like pumped storages. By using different technologies to cover Germany’s electricity demand, a new price curve is generated.

In an iterative process the load curves and the resulting price curves are exchanged between the MPC and the energy system optimization. It allows investigating the interdependent influence of changing load price curves.

The results will be analyzed, regarding the impact of energy flexible buildings on Germany’s electricity system (e.g. integration of renewables, development of storage and power plant capacities).Besides that, we will show how different building scenarios, for example high insulation versus high thermal activated mass, influence the result, regarding certain assumptions.

Optimizing the refurbishment of a single family home

Johannes Maderspacher[a], Thomas Auer[b], Werner Lang[c]

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Climate mitigation is one of the major challenges of our society. In Europe, the building stock is responsible for 40% of all energy consumption and 36% of total CO_2 emissions (EU-Council, 2010). Therefore, the refurbishment of existing buildings is a first priority measure when it comes to tackle climate change. Building energy simulation (BES) is a powerful tool/method to plan energy efficient buildings. But often, there is more than one objective to create an optimal building solution, e.g. reduction of energy consumption, global warming potential and the cost-benefits. Therefore, the application of numerical (multi-objective) optimization (MOO) in combination with building energy simulation can be useful. A possible drawback of these numerical optimizations is the computational effort. In this study we show that the substitution of a detailed building energy model with a neural network can strongly reduce the computational effort.

In a first step, a detailed building model of an existing single-family home is developed. After this a neural network is created based on the simulation results of the detailed model. Next a comparison of the meta model quality depending on the size of the learning set is carried out. For the optimization a genetic algorithm is used. To analyze the ability of the meta model for optimization the results are compared with a detailed building model. The neural network demonstrates the ability to replace a detailed building model for a multi-objective optimization. The neural network also demonstrates advantages in the computational effort for the optimization. For an MOO with 25000 simulations on a single core only 79 seconds are needed. For the same optimization a detailed building model requires 24 days.

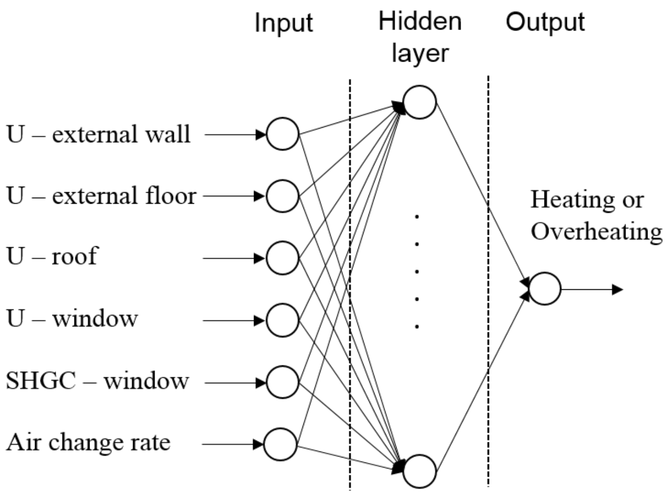

Figure 1: Schematic structure of the used neural network

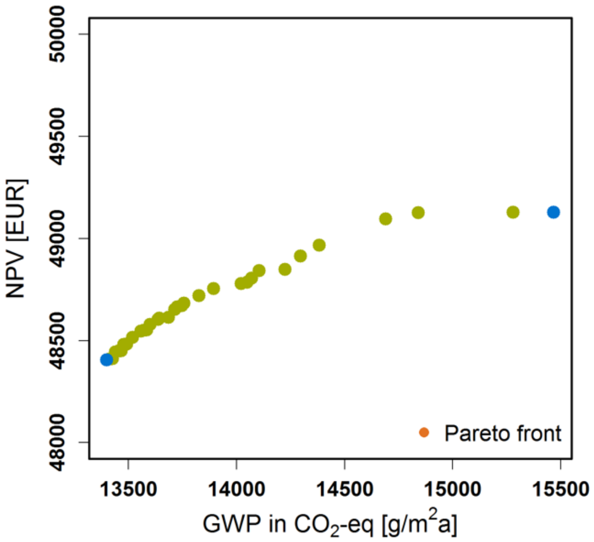

Figure 2: Pareto-optimal solutions of the multi-objective optimization of global warming potential (GWP) and net present value (NPV)

EU-Council 2010. Directive 2010/31/eu of the European parliament and to the council of 19 may 2010 on the energy performance of buildings. Official Journal of the European Union, pages 13–35

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Energy Management and Electromobility in Plus Energy Homes and Districts

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Heading for a near climate-neutral building stock, future buildings turn from energy consumers to prosumers. By actively using renewable energy sources in their envelopes and on the plot of land, modern buildings can generate more electricity and heat than their users need in terms of the total annual consumption. The energy surplus can serve as fuel for emission-free electromobility.

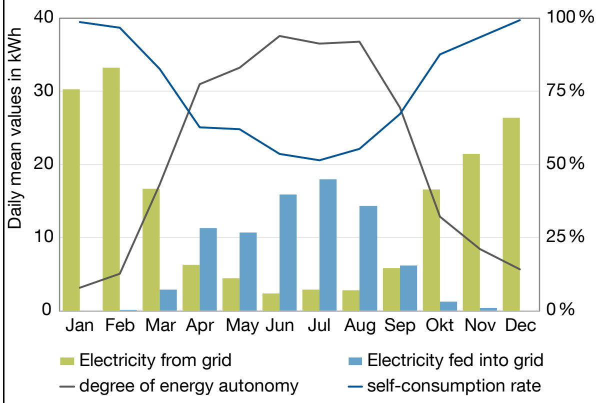

Figure 1: Self consumption and electricity exchange with the grid in the demonstration building

In the research project “e-MOBILie – Electromobility with autonomous energy supply in a smart micro-grid” TUM and several industry partners have developed an integrated energy management system, which intelligently connects energy-efficient building operation and solar-optimized charging of electric vehicles. The system was implemented in an occupied single-family plus-energy house equipped with a photovoltaic (PV) system, a heat pump and electrical and thermal storage systems. During the 1.5-years demonstration phase, solar electricity production, all energy flows and temperature levels in the building as well as electricity exchange with the electric vehicle and the public grid are subject to continuous measurement and analysis. The monitoring also includes an evaluation of the energy management system’s interactions.

The results show low impact of shifting loads like washing machine and dishwasher. For the electric vehicle, however, energy management raised the solar charging ratio from 3 % to 46 %. Hydraulic optimization of the heating system and the inclusion of the heat pump in the energy management improved the energy performance of the heat pump as the main consumer. Moreover, the PV self-consumption rate and the degree of energy autonomy significantly increased. Current work concentrates on a method to integrate e-mobility aspects into energy performance and sustainability certification of buildings.

Further studies analyzed the potential of PV systems as energy supply not only for individual homes but for multi-story residential buildings and urban districts with a growing number of electric vehicles. On one hand, the usable roof area per resident decreases with increasing number of stories and urban density. At the same time, the load profiles of the electricity and heat consumption and vehicle use become more homogeneous and the shifting potentials are greater. The combination of a large number of consumers generally enhances the use of fluctuating renewable energy sources.

Different energy demand and renewable supply scenarios were designed for multi-family houses of three different sizes and the two most common types of urban districts in Germany. Maximum possible PV installations as well as a rather moderate PV realization were taken into account to calculate the potential PV electricity production. Specifically developed models to simulate the consumption and charging profiles provide the potential PV self-consumption rates and degrees of energy autonomy for the scenarios. The calculations also identify the overall renewable energy surplus for e-mobility.

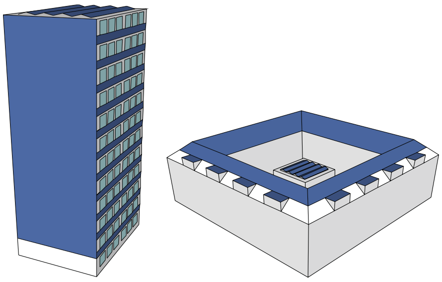

Figure 2: Analysis of PV potential in large buildings and districts

Metal electrodes in organic photovoltaics – why contact matters

Franziska C. Löhrer[a], V. Körstgens, M. Schwartzkopf, A. Hinz, O. Polonskyi, T. Strunskus,
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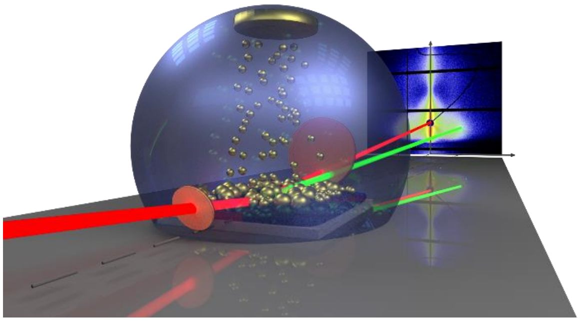
With a growing population and an increasing living standard, the world's demand for sustainable energy is rising. Alternative energy sources such as solar, wind or hydropower already contribute significantly to the energy supply in Germany [1]. However, they are typically limited to static, large-scale 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 surpassing the industrially important limit of 10 %. [2] However, they still show considerable efficiency losses and drastically decreased lifetimes 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 the interface between the photoactive layers of typical organic solar cells and their metal back electrodes.

Although OPV devices consist mainly of organic materials, their electrodes are in many cases still made from metals. Thus, polymer-metal interfaces are inherently present in these solar cells. We investigate the formation of the polymer-metal interface during the deposition of metal electrodes onto photoactive films via in-situ grazing incidence small angle X-ray scattering (GISAXS). [3] This technique allows for highly time-resolved insights into the deposition behavior of the metal on the organic film, which strongly depends on the film structure. The formation processes of gold contacts on different organic layers are compared. Further characterization techniques such as electron microscopy and UV/Vis absorption measurements complete our work. Understanding the deposition behavior of metal contacts on organic thin films plays a crucial role in identifying potential ways to enhance the performance of OPV devices.



Experimental set-up during electrode deposition

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[3] A. Hexemer, P. Müller-Buschbaum, IUCrJ 2, 106-125 (2015)

X-rays, Neutrons, and Positrons: Strong Contributors in Revealing Fundamental Processes in Lithium-Ion Batteries

Irmgard Buchberger[a], Stefan Seidlmayer[b], Markus Reiner[c], Thomas Gigl[c], Christoph Hugenschmidt[c], Petra Kudejova[b], Ralph Gilles[b], Michele Piana[a], Hubert A. Gasteiger[a]

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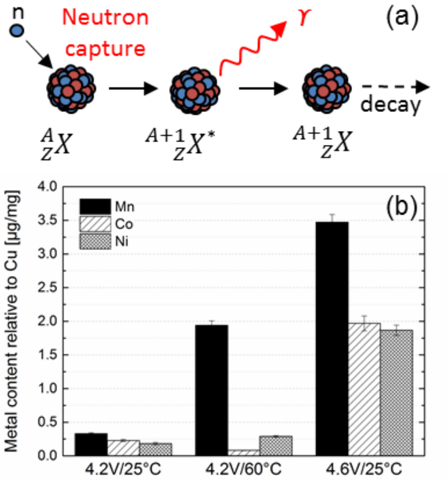

Figure 1: Neutron based Prompt Gamma Activation Analysis (PGAA) for quantitative and non-destructive detection of transition metal ions on graphite electrodes[1].

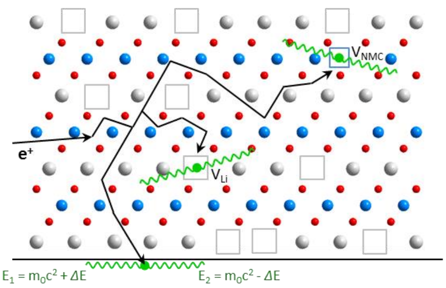

Figure 2: Positron annihilation spectroscopy (PAS) for the analysis of defect evolution and vacancy ordering in lithium-ion electrodes.

A full understanding of the operation of a battery requires the combination of investigative methods that are not always common. Conventional X-ray diffraction (XRD) has been a basic tool since the beginning of lithium-ion battery research and helped a lot in developing novel electrode materials and revealing insertion or degradation mechanisms. Over the years, such analysis has been supplemented by synchrotron or neutron-based techniques that offer higher resolution or sensitivity to certain elements.

Besides the common investigation of structural properties, neutrons can be further utilized in non-destructive quantitative elemental analysis. After activation of a sample by neutron capture, γ-rays are promptly emitted with characteristic energies that are specific for an element or isotope (Figure 1a). This method of Prompt Gamma Activation Analysis (PGAA) was successfully applied in an aging study on Graphite/$LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ (NMC) electrodes [1], in order to investigate and quantify the transition metal dissolution and deposition on graphite electrodes at different operating conditions (Figure 1b).

Furthermore, we recently analyzed the defect evolution of NMC during lithium extraction and re-insertion [2]. Positrons are very sensitive to open-volume defects, which can be easily measured by Coincidence Doppler Broadening Spectroscopy (CDBS). This method, applied for the first time on this material, proved to be very specific in analyzing the well-known kinetic-hindrance-effect observed close to the fully lithiated state during re-intercalation of NMC [3]. We also identified a distinct dependence of the Doppler broadening shape parameter S on the degree of lithium extraction and a correlation to the lattice parameter c of NMC.

In this contribution, the important use of X-rays, neutrons, and positrons in revealing fundamental processes in lithium-ion batteries is described. The focus is on the combination of conventional *ex situ* as well as *in situ* XRD with uncommon techniques based on PGAA and CDBS to shed light on major contributions to capacity fade and first cycle capacity losses.

[1] Buchberger *et al. J. Electrochem. Soc.* **2015**, *162*, A2737–A2746. [2] Seidlmayer *et al. First-Cycle-Defect Evolution of* $Li_{1-x}Ni_{1/3}Mn_{1/3}Co_{1/3}O_2$ *Electrodes Investigated by PAS,* in preparation. [3] Kasnatscheew *et al. Phys. Chem. Chem. Phys.* **2016**, *18*, 3956–3965

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Elucidation of adsorption processes at the surface of Pt(331) model electrocatalysts in acidic aqueous media

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The oxygen reduction reaction (ORR) belongs to the fundamental reactions of the renewable energy production. For instance, it plays an important role in so-called polymer electrolyte membrane fuel cells (PEMFCs) which due to their high power density and high energy conversion efficiency appear to be one of the most promising substitutes for future automotive industry. However, the sluggish kinetic of the ORR taking place at the cathode is still a factor which limits their performance and hinders the wider commercialization of these devices. Identification of specific catalytic centers as well as their nature, structure, relative surface abundance and electronic properties would enable an electrocatalyst optimization and as a result the PEMFCs' performance improvement.

Platinum is one of few materials providing high ORR activity, necessary selectivity and stability in acidic media usually required for modern PEMFCs. According to the commonly accepted models the most active sites are located at the Pt(111) facets, which bind reaction intermediates ~0.1 eV stronger than the optimal binding energy. Among many existing surfaces, special attention should be paid to Pt(331), known also as Pt[3(111) x (111)], which has long been found as the most active pure metal electrocatalyst towards the ORR in acidic media. Its activity appears to be ~4.5 times better than that of Pt(111) at the key electrode potential of ~0.9 V (RHE) for PEMFC applications, being even higher than several Pt-alloy electrocatalysts. Although multiple theoretical models mostly based on density functional theory (DFT) calculations have been elaborated, the exact origin of these experimental facts are still under discussion.

Based on the data obtained during cyclic voltammetry (CV) (Fig. 1) combined with potentiodynamic electrochemical impedance spectroscopy (PDEIS) in an O_2-free and O_2-saturated acidic media, we propose a model describing simplified adsorbate structures existing at the Pt(331) surface at different electrode potentials (Fig. 2). Even though the simulation seems to be highly hypothetical, it explains the CV and PDEIS data with a large precision. Nonetheless, the main results of the electrochemical studies are that ORR intermediates adsorption at the examined surface starts as early as 0.1 V (RHE) and that all steps at the potential of 0.9 V (RHE) are indeed blocked by oxygenated species. This leads to the further conclusion that the active sites for the ORR are situated at (111) terraces and supports the hypotheses indicating that the (111) facets are responsible for the high activity of many extended Pt surfaces.

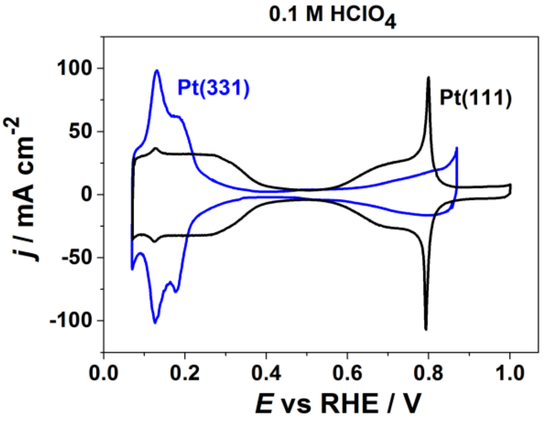

Fig. 1. Typical cyclic voltammograms of Pt(111) and Pt(331) in 0.1 M $HClO_4$

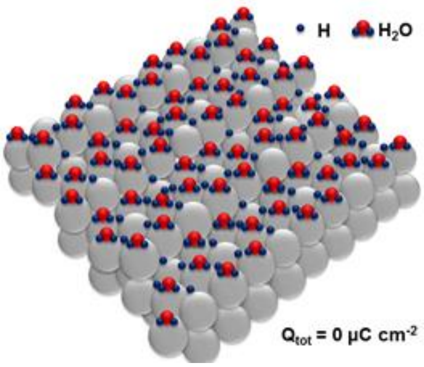

Fig. 2. Proposed adsorbate structure at the Pt(331) electrode surface developed during the oxidation sweep in the potential region between 0.05 V and 0.4 V (RHE)

Large-scale Power System Design - Improving Decomposition Techniques

Paul Stursberg[a]

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Across the world and particularly in Europe, energy systems are moving towards a significantly higher proportion of electrical power generated from renewable sources. This calls for new investment in the system infrastructure (e.g. transmission lines and storage facilities). At the same time, it poses new challenges to methods used to support and evaluate investment decisions: Investments are made with regard to a long time horizon, at the same time fluctuations in renewable generation need to be considered that happen on a timescale of minutes and are difficult to predict. In addition, the possibility to store power at a large scale means that the exact order of different load cases matters, thus rendering inadequate approaches that rely on the aggregation of similar load cases. Finding optimal investment decisions hence requires solving large-scale optimization problems within a reasonable timeframe.

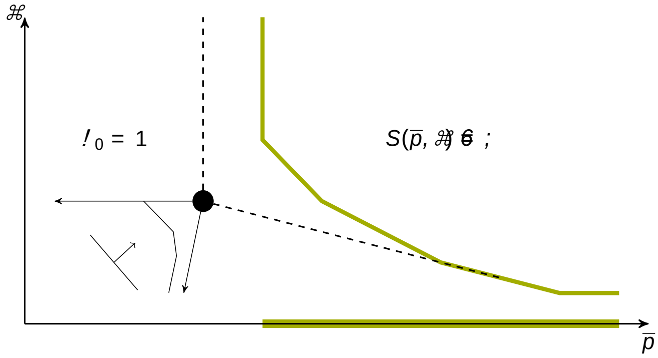

Figure 1: Set of feasible cut normals (bottom left) that separate current solution from the set of feasible solutions (top right)

For optimisation problems with a large number of variables and constraints, decomposition is a well-established technique to reduce the computational effort required to solve the problem. A large problem is decomposed into a master problem and several small, quickly solvable subproblems. Iteratively, information acquired in the master problem and subproblems is exchanged and for many approaches, finite convergence to a globally optimal solution can be guaranteed. One widely-employed approach is *Benders Decomposition*, where the information obtained from solving the subproblems is represented in the form of additional constraints (Benders cuts), that are iteratively added to the master problem. In this way, a representation of the subproblem cost as a function of master problem variables is built and iteratively refined. An important aspect of the design of Benders Decomposition algorithms is the selection of Benders cuts. While finite convergence can be assured for a large set of selection rules, the time required to solve the problem to optimality may vary by several orders of magnitude.

A number of methods have been proposed to select these cuts in a way that improves convergence to the optimal solution. Being designed for general mathematical programming problems however, these methods are unable to take into account much of the available expert knowledge and specific properties found in problems from the area of power system design. In our talk, we propose a number of improvements to existing cut selection criteria that specifically aim at exploiting structural insights into the problem in order to speed up the solution algorithm.

We present case studies to demonstrate that typical problems in power system design such as Transmission Capacity Expansion Planning can be solved faster to global optimality using the improved selection criteria. Furthermore, the approach opens up an avenue to make use of certain kinds of prior knowledge about the problem without compromising mathematical guarantees for the optimality of the computed solution.

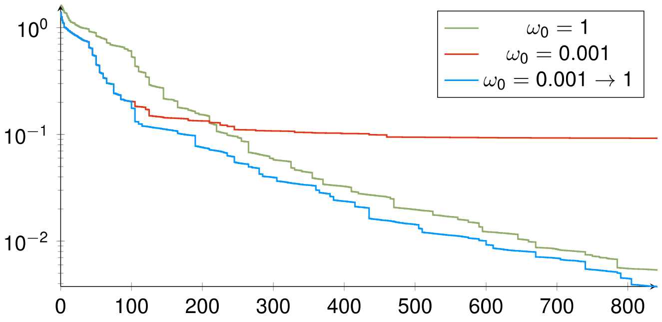

Figure 2: Relative optimality gap against iterations using different cut selection criteria

Towards fuel production from biomass *via* electrocatalysis and catalytic hydrogenation at ambient conditions

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Transportation fuels can be obtained from biomass-derived feedstocks using state of the art industrial processes. However, the production of high quality fuels requires gaseous H_2 to remove oxygen from the biogenic material. Whereas, H_2 may not be available in decentralized locations, excess electricity generated from renewable resources (e.g., photovoltaics, wind power, and hydropower) may be converted into chemical energy and stored in such biogenic feedstocks *via* hydrogen generated *in-situ* with electrolysis. Thus, coupling water electrolysis with the reduction of biomass-derived feedstocks, i.e., electrocatalytic hydrogenation of oxygenated compounds is an attractive alternative to upgrade bio-oil at mild conditions using carbon-neutral electricity.

This work investigates the electrocatalytic hydrogenation (ECH) and catalytic thermal hydrogenation (TH) of a variety of phenolic compounds and diaryl ethers, derived from deconstruction of lignocelluloses, on C-supported catalysts at ambient conditions. While TH is limited by ambient temperature and pressure, the rates of electrocatalytic hydrogenation (ECH) can be manipulated with the potential without alteration of ambient reaction conditions. At optimized conditions, the ECH rates can double those of TH (See figure 1).

Structurally simple compounds undergo hydrogenation towards cyclohexanones and cyclic alcohols at ambient conditions under ECH and TH. Increasing complexity of the reactants reduces their reactivity due to weaker interaction with the catalysts. However, functional groups in complex molecules undergo C-O bond cleavage. This opens pathways towards O-free hydrocarbons (drop-in fuels in the gasoline and diesel range), which can reach selectivity as high as 25 %.

ECH is sensitive to the nature of solvent and electrolyte due to the production of strongly adsorbing compounds at very negative potentials, which are needed in order to keep high currents in the presence of organic solvents. This problem can be circumvented by low-temperature coupling of TH and ECH. That is, performing ECH at optimum conditions and recycling the evolved H_2 (ex-hydrogen evolution reaction) to increase the contribution of TH. Hence, this work advances our understanding of the low-temperature conversion of biomass and allows identifying the main challenges for technological realization.

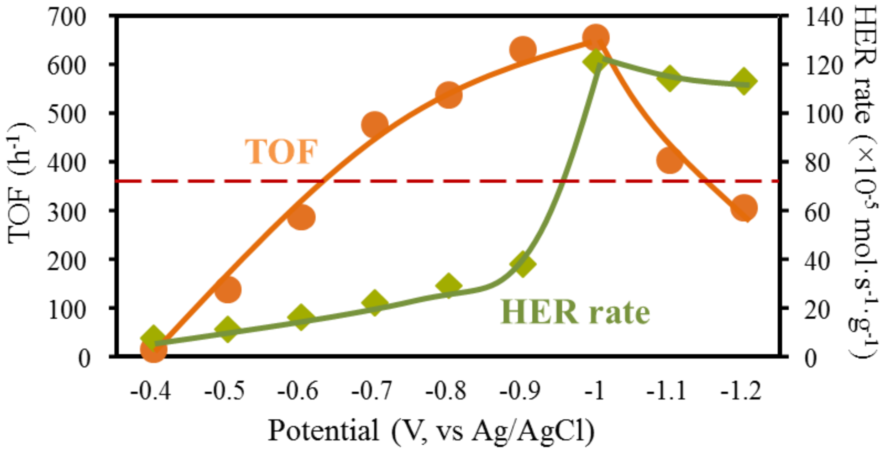

Figure 1: Rates of electrocatalytic conversion of the model compound phenol (TOF, orange line) and the H_2-evolution reaction (HER, green lines) in function of applied potential. The rates of electrocatalytic conversion can be tuned to rates higher than that of thermal hydrogenation (represented by the red dashed line). Decreasing activities at potentials more negative than -1 V can be compensated using the H_2 from HER.

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Optimal feedforward control of permanent-magnet synchronous machines in renewable energy systems

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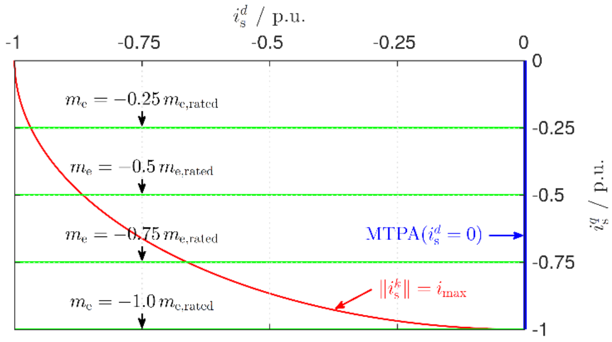
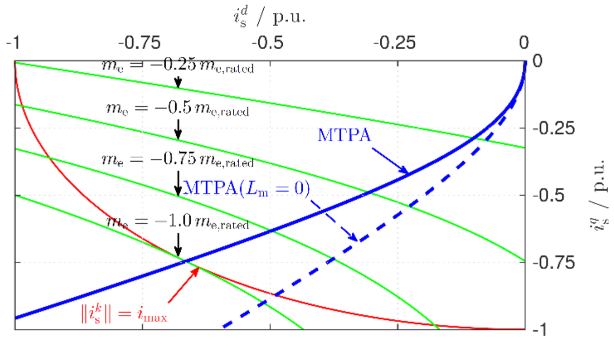
This talk will discuss *analytical* solutions for the optimal feedforward control problem (e.g. Maximum Torque per Ampere (MTPA) or Maximum Torque per Volt (MTPV)) of synchronous machines (SM). For the derivation of the analytical solutions the considered synchronous machines may exhibit anisotropy, magnetic cross-coupling and non-negligible stator resistance(s).

For a given reference torque, the analytical MTPA or MTPV solutions provide the optimal stator current references which will produce the desired torque while the stator copper losses or the required stator voltages are minimized. Hence, efficiency or voltage use will be increased by simple feedforward control. From an implementation point of view, the proposed analytical solutions are appealing in terms of its fast online computation (compared to conventional numerical methods). In particular, the efficiency of the analytical MTPA operation, with and without consideration of the cross coupling, will be compared to conventional feedforward control methods (e.g., zero direct current, see figures below). The negative effect of neglecting the stator resistance on the MTPV solution will also be illustrated.

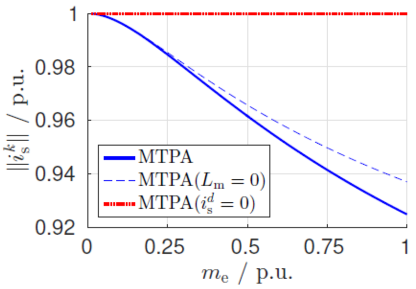
Concluding, to the best knowledge of the authors, the presented analytical solutions have not been reported in the literature this far. Moreover, most available methods impose simplifying assumptions to obtain (numerical) results leading to (possibly very rough) approximations of the optimal stator reference currents and, hence, to an overall control performance which is *not* optimal.



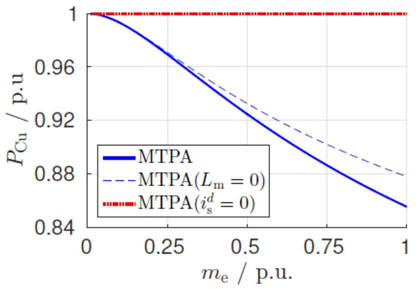
(a) *Isotropic machine:* $m_e(\boldsymbol{i}_s^k) = \frac{3}{2}\psi_{pm} i_s^d$.



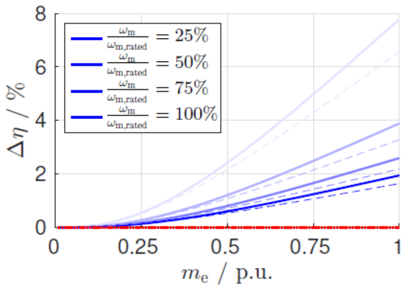
(b) *Anisotropic machine:* $m_e(\boldsymbol{i}_s^k)$ *as in* (1).



(a) *Current magnitude*



(b) *Copper losses.*



(c) *Efficiency improvement.*

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OpenGridMap: Automatic Power Grid Simulation Model Generation from Crowdsourced Data

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OpenGridMap (opengridmap.com) is an open-source project that crowdsources realistic power grid data to be used for research purposes.

The energy transition requires substantial changes to the current electric power transmission and distribution infrastructure. Several solutions to support the energy transition are currently being researched. Solutions range from a significant expansion of the current transmission and distribution capacity, to the introduction of new devices such as distributed generators, distributed storage units and electric vehicles. To properly assess the technical, economic and social impact of the proposed solutions, researchers will need to run complex simulation studies using realistic data. Currently, simulation studies for power grids rely heavily on standardized test grids, e.g., the IEEE test feeders, the CIGRE test feeders, and the PNNL feeders. Although these test cases are often used and have certainly contributed to the reproducibility, and thus the comparability, of research results, it is important to point out that they represent an average of how power grids are. In reality, power grids can be highly individual, e.g., due to geographic features, utility strategies, regional legislation, or simply coincidence. Hence, the ability to do simulation studies based on realistic data can improve the quality and applicability of proposed solutions. The problem however, is that the availability of realistic input data for such simulations is very limited. To this date, there is no resource available that allows researchers to obtain structured power grid data for a particular geographical region, let alone a simulation-ready model for the power grid of a particular area. With the OpenGridMap we want help fill this research gap.

In this work we propose an approach for the automatic generation of power gird simulation models from crowdsourced data. The proposed approach orders the crowdsourced data into a power circuit relation which is then used to produce a CIM description file and subsequently a simulation-ready power grid MATLAB Simulink model. We provide experiments which demonstrate the effectiveness of the approach on OpenGridMap data. Given the large amount of crowdsourced data available, our approach has the potential to generate power grid simulations of larger size, more variety and more accuracy than the currently available state-of-the-art test power grids.

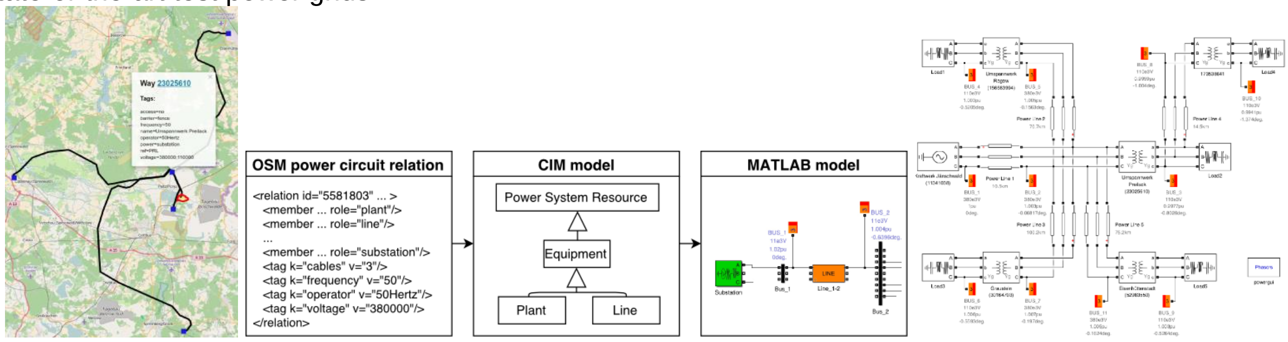

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Fig. 1: From crowdsourced data to simulation-ready Simulink model.

Flexible Power Generation with Thermal Power Plants: Process Analysis Using Dynamic Simulation

Steffen Kahlert[a], Julia Hentschel[b], Hartmut Spliethoff[c]

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On the road to a decarbonized economy thermal power plants play an essential role. The share of electricity produced by fossil-fueled power plants must be decreased continuously. Still, there is a demand for back-up capacity because of intermittent renewable generation. Thus, the operation regimes of existing power plants have to be modified considerably. The flexibility is an important requirement of thermal power plants. They must operate with high load gradients in a wide load range to support the integration of renewable energies. Due to numerous operational restrictions, a thorough process analysis is essential to maintain operational safety during transient operation.

In the course of the MSE project "Energy Valley Bavaria - Flexible Power Plants", a dynamic process simulation is performed for both coal fired power plants and combined cycle power plants in cooperation with power plant operators. In the first step a detailed process model is developed on the basis of design data and validated with operational data. The next step is the identification of limiting factors in the control system regarding the flexibility. This could be e.g., predefined maximal load gradients based on a former conservative estimate. During the optimization process, the simulation model is used to tune control parameters, to modify the architecture of the control loops, and to investigate the effect of faster load gradients on the lifetime of critical components.

Secondary control reserve (SCR) represents the load change that can be performed in five minutes and poses high demands on the controllability of the load. Regarding the simulation of coal fired power plants, a model was successfully developed to identify necessary control modifications for an increased SCR supply.

In comparison to coal fired power plants, combined cycle power plants have superior dynamic characteristics because the gas turbine is able to perform high load gradients. A dynamic simulation model of an industrial power plant is presented that provides electricity and heat for an industrial consumer. Both the electrical load and the thermal load must be altered quickly. The maximum amount of secondary control power and the impact on the process stability is analyzed. The load range is limited by the operational restriction of the gas turbine, the supplementary firing and the steam turbine. The feasible load change depends on the steam flow that is extracted from the steam turbine. Furthermore, the supplementary firing is responsible for avoiding large control deviations of the live steam pressure by compensating the thermal inertia of the heat recovery steam generator. The analysis shows that the existing control system is not able to maintain stable process parameters during high load gradients. A model based control is implemented in the simulation model and shows an improvement of the process stability during dynamic operation.

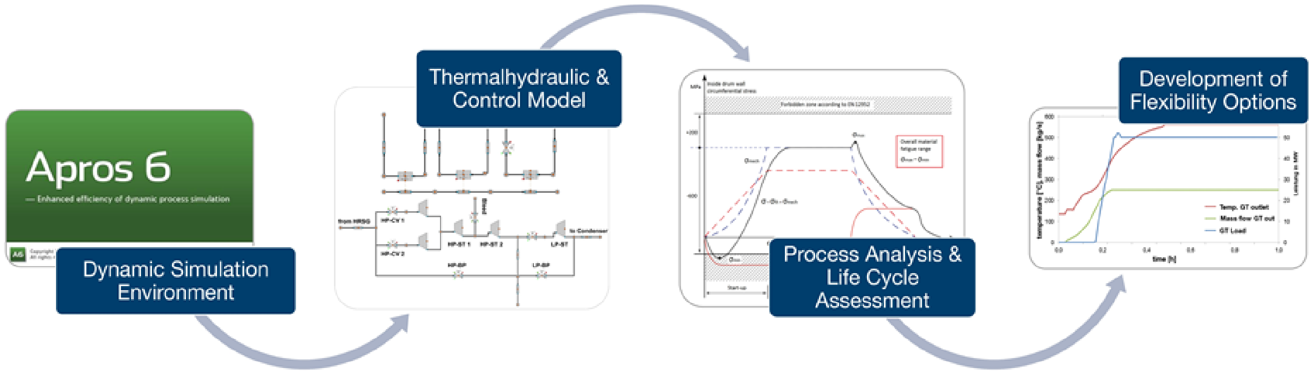

Figure 1: Methodology for the usage of dynamic simulation models in optimization processes for thermal power plants

Wind farm control for power maximization

C L Bottasso[ab*],
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*carlo.bottasso@tum.de

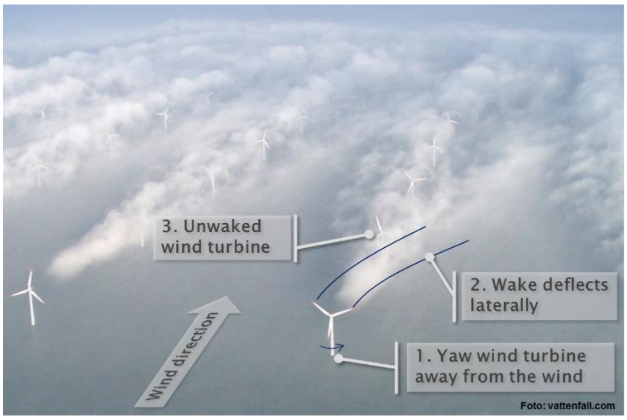

Figure 1: Concept of wind farm control by wake redirection

Wind turbines extract kinetic energy from the air flow, transforming it first into mechanical and eventually into electrical energy. Because of this energy extraction and conversion, the wake shed by a wind turbine is characterized by lower speeds and higher turbulence intensity than the freestream. Wind turbines are often clustered in wind farms in order to reduce land occupation and connection costs, improve logistics and maintenance, limit impacts, and for various other reasons. Hence, for certain wind directions, wakes shed by upstream wind turbines can shadow downstream machines, resulting in yield losses and increased fatigue loading.

In this work we consider the solution that currently appears to be the most promising one, namely wake redirection. The idea is to deliberately point the upstream wind turbine slightly away from the incoming wind direction. While the power capture of this wind turbine will be reduced, a misalignment with the wind will also to some extent displace the wake laterally. As illustrated in Figure 1, one can use this technique to deflect the wake away from the affected downstream machine, reducing or eliminating altogether the negative shadowing effects, in turn increasing power capture on that wind turbine. If the gains on the downstream wind turbine exceed what is lost on the upstream one, it is clear, that the total power output of the two machines will be greater. The same cooperative control concept applied to the whole wind farm might result in significant yield increases A similar strategy could also be used for finding an optimal compromise between power capture maximization and load alleviation.

Figure 2: Scaled wind farm

The team of the TUM Wind Energy Institute approaches wind farm control through sophisticated CFD-simulations, the development of methods for wind and wake estimation based on rotor loads, as well as wind tunnel experiments. By connecting all the approaches above, we could recently show for the first time that the described control concept can be successfully implemented in closed-loop manner on a scaled wind farm operated in a large boundary layer wind tunnel (see Figure 2). Results indicate a significant increase in wind farm power exemplary shown in Figure 3. With a LiDAR system the wind speed inside the entire wind farm could be measured. The visualization in Figure 4 shows the wake deflection (at right) compared to the wind farm without cooperative control (at left).

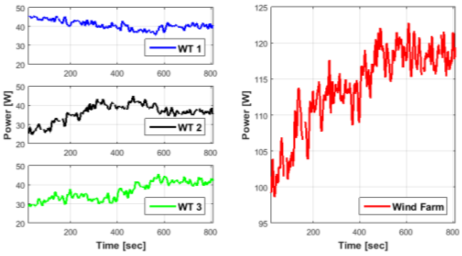

Figure 3: Time histories of the individual turbines (at left) and the entire wind farm (at right)

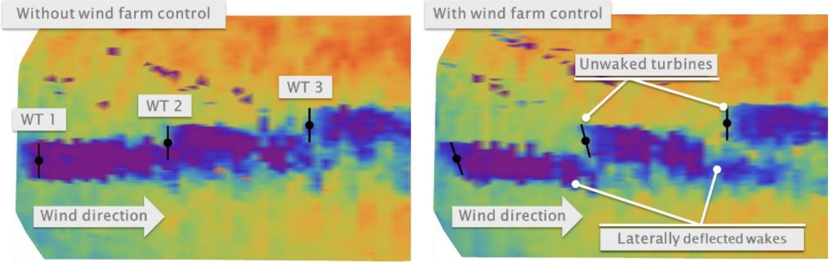

Figure 4: LiDAR plan view of the wind farm showing the undeflected wakes (darker color) (at left) and the deflected wakes through upwind turbine yawing (at right)

2 Poster presentations

Stability of *in situ* polymerized polythiophene in organic solar cells

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Solar cells are devices that transform sunlight to electricity through the photovoltaic effect. The standard and commercially available solar cells are made of silicon. These are expensive mainly because of the high cost of production. In comparison to that, organic solar cells represent an alternative that could make solar cells financially accessible to more people around the world. The employed polymers can be fabricated from solution, making large scale and low cost production techniques like printing possible.

Organic solar cells can have one of two main device geometries: the standard and the inverted geometry. In the standard geometry the layer stack is usually built on top of a semitransparent indium tin oxide (ITO) electrode followed by a hole transport layer (PEDOT:PSS), the active layer (electron donor and acceptor), an electron transport layer and finally a low work function metal electrode (the cathode). In the inverted type geometry, the order of the layers is reversed with the top metal electrode now being the hole collecting anode.

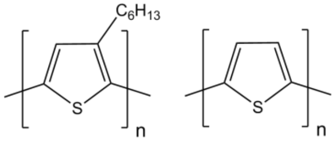

Figure 1: Chemical structures of P3HT (left) and polythiophene (right).

Polythiophene is a semiconducting polymer with a conjugated backbone which may become conductive upon doping. Since polythiophene is insoluble in most solvents, it needs solubilizing alkyl side chains in its chemical structure to make it solution processable. Here, we present polythiophene synthesized in situ by a chemical oxidative polymerization reaction of bithiophene. This way, we obtain solution processed thin films of a semiconducting polymer without electrically insulating side chains.

Nevertheless, two of the most important disadvantage of the organic solar cells are their lower efficiency compared to silicon devices and their shorter lifetime and material stability. Chemical degradation of organic solar cells is mainly caused by oxygen, water and electrode material reactions with the active polymer layer.

In this work, we investigate the stability of polythiophene under different conditions. For this purpose, we synthesize polythiophene thin films and measure their optical (absorbance measurements) and electronic (conductivity and charge carrier mobility) properties.
Moreover, we look at the performance of polythiophene:PCBM solar cells and the ageing of the active layer materials. The investigated solar cells are built in an inverted geometry, to ensure a long lifetime and stability of the other components.

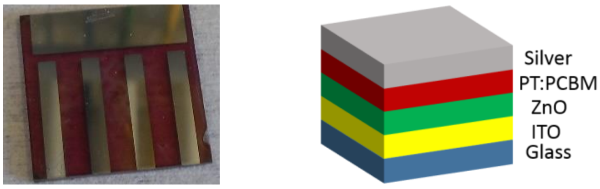

Figure 2: Image of lab-scale organic solar cell (left) and schematic diagram of layer stack of inverted geometry (right).

References:

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2. M. Jorgensen et al., “Stability of polymer solar cells”, Adv. Mat., 24, pp. 580-612, 2012

Kinetic Parameter Estimation of Lithium Ion Battery Active Materials

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Lithium Ion batteries (LIB) are an important technology as they are an ideal candidate for a variety of applications due to their high energy, power density and operating voltage. In order to use LIB systems efficiently a good understanding of their performance over a range of operating conditions is necessary. While simulation and modeling, which allows optimization of design and control, can be useful to predict battery behavior they require precise knowledge of a large set of physical and chemical parameters of the system[1]. Among these parameters a detailed knowledge of the charge transfer kinetics of the lithium intercalation reaction is crucial for design and optimization of advanced active materials. However in the literature coarse simplifications are made to describe kinetics[2] or kinetic parameters are fitted to match experimental data[3]. Consequently, there is no good agreement between model predictions and experimental results or the significance of computational studies is limited by the accuracy of the parameters used. Experimentally there are lots of difficulties concerning the investigation of charge transfer kinetics of lithium intercalation in LIBs due to which there is only little research work in this field[4]. In order to provide precise and significant simulation results the used parameters have to be determined accurately.

In the work we are presenting, we show a unique method that we have developed to reduce the uncertainty in estimating the kinetic parameter of the active materials. We use Swaglok three electrode cells with $LiFePO_4$, $LiNi_{0.33}Mn_{0.33}Co_{0.33}O_2$ and $Li_4Ti_5O_{12}$ as working electrodes with metallic lithium foils as both counter and reference electrodes. For each active material current pulses of 2s duration are done for a range of discharge currents and the corresponding potential transients are recorded. We processed and analyzed the data using MATLAB and found that for smaller current pulses the charge transfer resistance can be obtained easily by extrapolating the plateau of the potential profile. At higher current pulses the total overpotential is dominated by concentration overpotentials resulting in non-stationary potentials during the measurement.

To extract the activation overpotential from the total overpotential at higher current pulses we apply 1D LIB model in COMSOL using concentrated solution theory and a surface reaction term. The parameters required to model the electrolyte solution in 1D LIBs were obtained experimentally in previous works[5,6]. Latter works allow us to solely identify the kinetic parameters by correlating experimentally obtained transients with simulations.

Our work will give new and deeper insight into the charge transfer kinetics of lithium ion batteries, thereby enhancing the reliability and significance of widely applied numerical investigations. Consequently, active materials and electrodes can be developed specifically to increase the performance and the lifetime of current and future lithium ion batteries.

Acknowledgement

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Effect of temperature on the electrochemical performance of Li-ion batteries and the structure of electrode materials

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Lithium-ion based electrochemical energy storage technology possesses a number of advantages (when) compared to its alternatives, e.g. in terms of self-discharge, high voltage, high energy and power densities, good cycle life and excellent storage characteristics. Despite their overall success, further research on Li-ion batteries towards higher energy/power density, lighter weight, safer and lower cost rechargeable batteries is of high scientific and technological relevance [1]. There is also another aspect to be addressed: the stability of the Li-ion cells over a broad range of environmental conditions, where operating temperature is one of the most important criteria. According to the recommended range of Li-ion battery operation (0 - 100°C) their use in countries with hot and frigid climate becomes somewhat bounded. Limited low temperature performance of Li-ion batteries turns out to be even more critical in aerospace applications, where stable energy storage and conversion under more extreme environmental conditions is demanded over a long period of time. Therefore, broadening the temperature range of stable battery performance is an emergent research task.

In literature diverse and somewhat contradictory opinions about the origin of the limited performance of Li-ion batteries at low and high temperatures can be found. However, the role of electrode materials, especially of electrode structure on the cell performance at different temperatures was poorly studied, i.e. no comprehensive electrochemical and structural studies of lithium ion batteries at both low and high temperatures were found. This can be related to the fact that despite the relatively simple principle of operation modern Li-ion batteries are sophisticated electrochemical devices possessing numerous degrees of freedom and complicated interactions dependent on chemistry, morphology, packing density etc. Their accurate identification and study requires experimental approaches capable to give information about processes occurring “live” inside the battery thus eliminating the risks of possible materials oxidation, electrolyte evaporation and battery state-of-charge changes. Among different experimental methods capable to probe the structure of Li-ion cell constituents under real (also non-ambient) operating conditions neutron scattering is already a well-established tool having numerous advantages [1-2]. The most prominent one is the high penetration depth of thermal neutrons enabling non-destructive studies of commercial Li-ion cells.

Operating temperature is the key factor determining kinetics, performance and stability of a Li-ion cell. Other cell parameters (typically optimized at ambient temperature) might be affected by temperature as well. The role of temperature on the depth of discharge, accessible cell capacity and discharge time has been shown in Ref. 2. Another important factor is the mismatch in thermal expansion of various constituents of Li-ion cell, which may lead to mechanical stress and, thus, affect its stable operation and performance. In the current contribution we report combined in situ electrochemical and neutron diffraction studies on Li-ion batteries of the most common design (18650-type, based on $LiCoO_2$ as positive and graphite as negative electrode). Temperature-resolved studies were performed over a broad temperature range (-123 – 100°C) on cells in charged and discharged state. In situ structure evolution of cathode and anode at different lithiation states was determined and analyzed in terms of cell integrity and performance.

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Design of a meteorological station for island-grids

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Figure 1: Solar Water Pump (Zimbabwe)

Motivation

Island-grids using renewable energy can play a major role in the electrification of rural areas in developing countries, particularly in Sub-Saharan Africa. The design of island energy systems is subject to several technical and economic constraints, such as reliability and cost-competitiveness. In remote rural areas, additional aspects (e.g. robustness, user-friendliness, availability of materials, reliability of data) need to be taken into account. Current research is undertaken in order to design island energy systems that comply with these stringent requirements while providing economically viable solutions.

Technical implementation

The lack of reliable long-term meteorological data in Sub-Saharan Africa, which are necessary for system sizing, has encouraged our research group to design a low-cost meteorological station that can be used in remote areas in developing countries. The meteorological station uses a Raspberry Pi system as a data logger for long-term acquisition of wind speed, temperature and solar radiation data. The “upload” function saves the files into a cloud folder, whereas the “delete” function cleans the storage space by removing old files. On-site experiences in Banket, Zimbabwe showed that the most important aspects for the product design are the self-sustaining energy supply and the data transfer via SIM-card. Continuous field testing has led to further improvements on the prototype.

Figure 2: Raspberry Pi

The role of the meteorological station will not be limited to acquiring reliable data for site prospection. Once island energy systems will be installed in remote areas, they will include a meteorological station that will measure wind speed, temperature, solar radiation, humidity and precipitation. In order to provide accurate and reliable measurements, the meteorological station prototype complies with the norms that regulate the measurement of weather parameters, while being compact and mobile.

Long-term goals

The long-term idea is to use the measurements as well as historical data to predict the weather for the next hours. On the one hand, the weather forecast can be used in combination with the load forecast and the battery monitoring system to optimize the operation of the island energy system and improve the battery life. A micro-controller processing the aforementioned data through a suitable control algorithm could be an effective solution to the intermittency of renewable energy sources and is expected to decrease total system costs. This hypothesis will be assessed in detail in a later stage. On the other hand, the weather prediction can be offered as a service for the village where the meteorological station is installed. A market potential assessment for island energy systems using meteorological stations is still ongoing.

Network Design and Yield Optimisation of Solar District Heating Systems for Urban Applications

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Multi-storey residential buildings provide high potential for solar-assisted local district heating. Current research projects focus on the utilisation of large seasonal storages to achieve a solar fraction of above 50 %. However, for retrofitting densely built-up urban areas, the feasibility of solar district heating is often restricted by the limited space available for collector arrays and heat storages. Moreover, high storage capacities come with high investment and heat production costs. These drawbacks impede the applications of seasonal storage concepts in existing urban areas and hinder the dissemination of large solar-thermal systems.

This project aims to tackle these challenges by investigating a novel solar district heating design based on distributed solar collector arrays and thermal heat storages in multi-storey residential buildings with bi-directional heat distribution capability and the intelligent interaction of these components. The study will examine the network design and yield optimisation of such a system in various urban contexts.

Focus of this contribution is the investigation of a real district heating network in Ingolstadt. Under the given boundary conditions of this object (e.g. roof size, orientation and available space in the basements of the buildings), solutions for different ways of utilising solar heat were found. Based on a simulation study in MATLAB/Simulink, using the CARNOT-toolbox, these different solutions were optimised regarding hydraulic layout and plant size.

Three different plant types are currently realised in four buildings of the investigated object. These provide either a local use of the solar gains, a pure feed in to the district heating network or a combined solution. Annual solar yields between 280 and 660 kWh/m² are reached in the simulation. A concept for the metrological investigation of these plants was developed. This includes the logging of relevant heat fluxes in the buildings, where the solarthermal plants are set up and the installation of energy meters in every substation of the district heating network to get a complete energy balance of the system. Throughout the year, a detailed acquisition of the measured data will be conducted. This allows, besides the comparison of the different plant types, the validation of the simulation model. After this validation, an adaption and, if possible, a simplification of the model will be performed as basis for further simulation-based optimisations.

Figure 1 shows the district heating system with the positions of the new solarthermal plants and the additional energy meters in the substations.

The findings of the study will show whether the intelligent interaction of the system components can adequately compensate for the lack of storage capacity as compared to the seasonal storage concepts. The outcome of the project can contribute to the realisation of renewable heating systems with low solar heat costs in combination with a decent solar fraction.

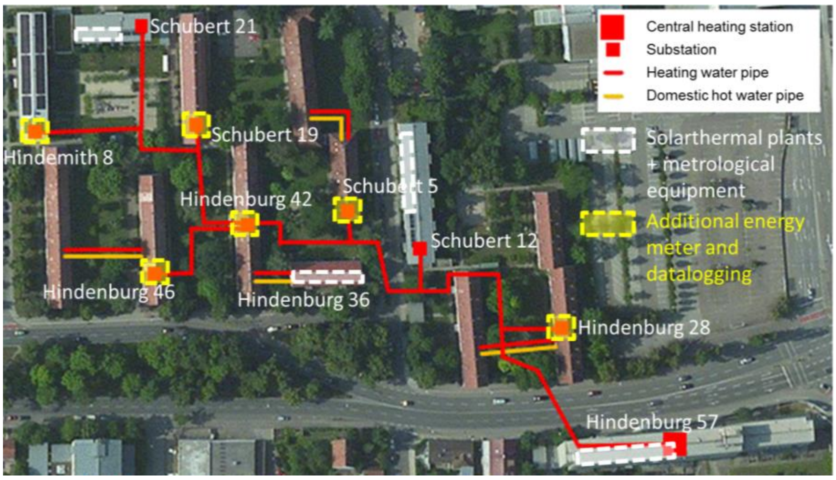

Figure 1: Investigated district heating system with positions of solarthermal plants

Investigation of Active Material Distribution in an Operating Lithium Sulfur Battery Using Spatially Resolved Operando X-ray Absorption Spectroscopy and Fluorescence Mapping

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To meet the increasing demand of lightweight energy storage possibilities for electric vehicles or wearable technologies, new battery solutions with promising high energy densities like lithium sulfur batteries are currently being investigated. One of the major obstacles in a way of wide-spread commercialization of lithium sulfur batteries is the polysulfide dissolution which results in loss of active material [1]. Therefore, much effort has been made to either trap the polysulfides in the cathode material [2] or to create a physical barrier, preventing them from diffusing to the anode side [3].
To date, however, there has been little analysis of the exact dissolution- and diffusion processes in correlation with their time- and voltage dependence. Therefore, it was our goal to track the location of the sulfur during operation of the battery to develop a better understanding of the distribution of the material inside the battery.

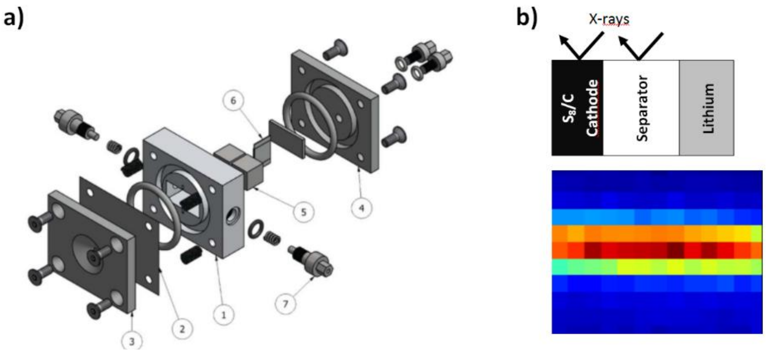

Figure 1: a) Exploded view of the spectro-electrochemical cell: (1) cell base; (2) X-ray window; (3) and (4) aluminum front-plate and back-plate; (5) stainless-steel current collectors; (6) electrode-separator assembly; (7) stainless-steel electric contact pins; b) Demonstration of spatial resolution; x-ray fluorescence mapping during open circuit voltage of the cell: sulfur signal ordered in S_8-cathode

We have used a unique cell setup (Fig. 1a) that has been developed in our laboratory [4]. This cell setup allows spatially resolved measurements of the two essential spots of an operating lithium sulfur battery: the sulfur-based cathode and the separator. Using operando x-ray fluorescence mapping, we were able to track the location of the sulfur compounds throughout the cell. In combination with operando x-ray absorption spectroscopy, we could additionally determine the chemical composition of the sulfur species present in the analyzed two locations of the cell. The initial mapping is demonstrated in Figure 1b, in which the sulfur signal is initially ordered in one stripe in the S_8 cathode. During the charging and discharging processes, we could detect the location and the composition of the forming intermediates at all times resulting in a detailed set of data that allows a deeper understanding of the lithium sulfur cell chemistry.

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Designing nanostructured scattering layers for OLED applications

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Figure 1: Example for room lighting (Osram)

In the last years the efficiency and the life expectancy of organic light emitting diodes (OLEDs) reached values which make them suitable for industrial applications. OLEDs are able to cover a wide range of the color spectrum due to a large variety of different organic emitters. Combined with high color rendering and their energy saving potential, OLEDs became of high interest not only for display manufacturers.

Additionally, OLEDs are based on thin-film technology which makes the device – depending on the substrate – transparent and flexible. Moreover, the production is also less energy demanding. As a consequence, OLEDs enable new possibilities in energy saving, e.g. for room lighting.

The research was mainly focused on the internal quantum efficiency to enhance the conversion of electrical power into light which makes OLEDs much more efficient. By using phosphors the internal quantum efficiency reached values close to 100%. However, the extraction of photons out of the device is still a limiting factor, especially for white OLEDs. For conventional device architecture approximately 80% of the generated photons are trapped in the device and are eventually absorbed. Hence, there is still a high potential for the enhancement of OLED efficiencies by increasing the photon extraction.

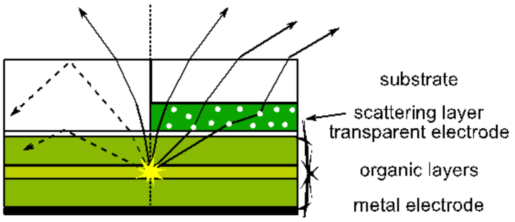

Figure 2: Basic principle of an additional scattering layer

There are several approaches to increase the photon extraction which are based on adding scattering centers into the device. Besides the direct structuring of the substrate surface, the attachment of a transparent layer on the substrate is a very promising approach.

Among the different possibilities to create scattering centers in such transparent layers, a nanostructured metal oxide layer holds high potential because of its high stability and its high refractive index.

With an optical band gap of 3.3 eV and a refractive index of 2.0, zinc oxide (ZnO) is a very promising material for this approach. The obtained ZnO layers are transparent for visible light and provide high diffuse scattering. Thus, these layers hold the possibility for redirection of the generated photons in an OLED device and should be able to enhance the photon extraction and the overall device efficiency.

In this work a structure directing diblock copolymer is used as template and combined with sol-gel chemistry for tailoring the ZnO scattering layer. This yields thin films with a well-controlled nano- and micro-structure.

In order to achieve a suitable film thickness, spray coating is chosen as the deposition technique for the prepared solution. The film morphology as probed by scattering techniques and electron microscopy is related to the spectral response to gain a structure-function relationship.

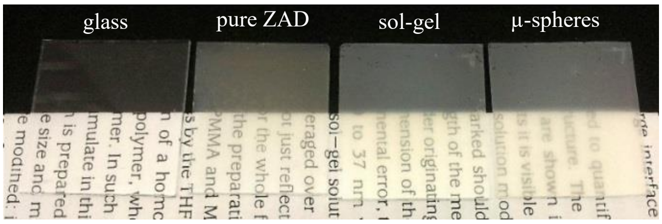

Figure 3: Differently processed ZnO scattering layer on glass substrates

Bayesian Networks in knowledge based occupant behaviour modelling

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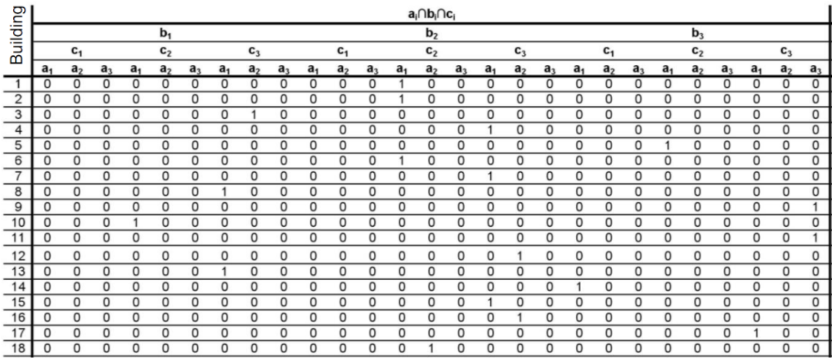
Status Quo: Latest data indicate that the EU will not achieve its energy-efficiency goals if only technology-oriented strategies are deployed. The enormous energy saving potentials in buildings cannot be fully utilized with ignoring the human dimension. Recent studies show that user behaviour can account for high variances in heat, electricity, and water consumption. With constantly improving building standards, the influence of the occupant on the building energy consumption will even increase. It is crucial to include detailed user behaviour models in early stages of planning and building design as well as in energy feedback and energy audits.

Methodology: A parameter study will identify the most influential behaviour characteristics of building occupants, providing detailed actions and background information for databases. An ongoing assessment of scientific studies, literature review accomplished with own simulations and building models will create a dataset of various occupant behaviour patterns. These patterns then are weighted and brought into causal relations and dependencies. In order to couple this information with the physical building model a Bayesian Network is used.



Building	$a_i \cap b_i \cap c_i$																										
	b_1									b_2									b_3								
	c_1			c_2			c_3			c_1			c_2			c_3			c_1			c_2			c_3		
	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3	a_1	a_2	a_3
1	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0
6	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
8	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
10	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1
12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
13	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
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16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
18	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0

Figure 1: Database with causal relation of various building parametes [Mavrioudi 2015]

Bayesian Networks:
The mentioned network needs to be able to combine the reliable information of the user databases with the uncertain, general information of standards and norms. In the Bayesian-Network (BN) the different parameters are set in causal relation to each other and the related uncertainties and probabilities of occurrence of occupant actions are calculated dynamically. The results of that step persist of behaviour patterns, which change their weight and values depending on the evidence of the personal input data of the occupant. These patterns will then be transformed into scripts and text files, which can be read by the physical building performance simulation environment. The behaviour itself will be translated into schedules and activities which regulate the amount of internal heat gains, ventilation behaviour etc.

First Results: Our first simulations indicate that the energy demand of an occupant behaviour based building model varies up to 75% compared to the deterministic results of simulations based on norms. Depending on the occupant behaviour the energy demand is calculated 5% below the average standards, when considering the worst behaviour additional 35% of energy demand are calculated. Additionally, a first overview over the various behaviour parameters was created. It is basically a graphical depiction of behaviours and how they are related to each other.

Hybrid solar cells with laser-ablated titania nanoparticles

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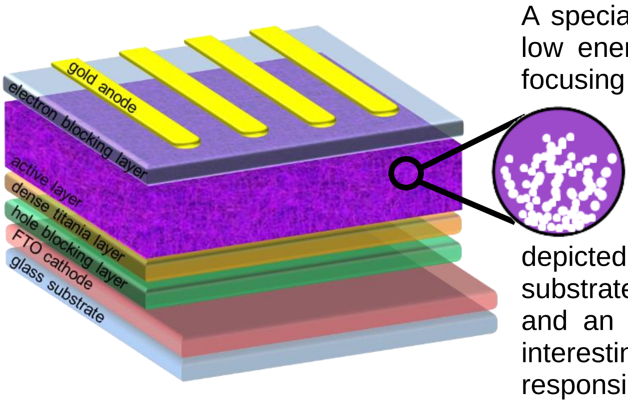
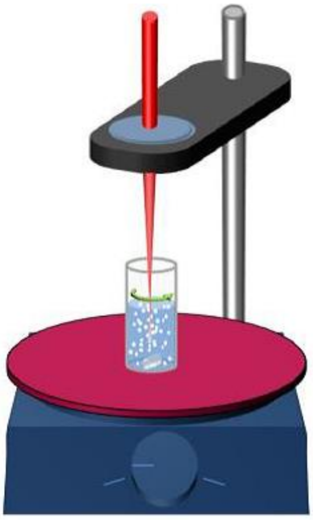
Hybrid solar cells are a promising technique for future energy generation as they combine the advantages of organic and inorganic solar cells. Organic materials are solution processable. Therefore, they enable large scale and cheap production with little energy demand. They also allow for thin film devices sparing scarce resources. Furthermore lightweight and flexible cells are suitable for new applications. On the other hand the usage of inorganic material like titanium dioxide (titania) provides high charge carrier mobility and avoids degradation.



A special emphasis lies on environmentally friendly, cheap and low energy production routes. In that regard our approach is focusing on a completely water based hybrid solar cell. As depicted on the left image, it consists of an FTO-coated glass substrate with different layers: a titania hole blocking, the active and an electron blocking layer with gold contacts. Especially interesting is the active layer of the solar cell because it is responsible for the light absorption. Our system consists of a bulk heterojunction formed by titania nanoparticles as an electron acceptor and a hole conducting polymer as an electron donor.

One method to produce the titania nanoparticles is laser ablation in solution [1], shown in the right picture. It is a water based process and a low temperature process, thereby reducing the energy demand. The base material for the ablation process is titania powder, because it provides a higher generation rate of nanoparticles as compared with a solid titanium target. The titanium dioxide can be functionalized by the water soluble and thiophene based polymer P3P6T [1]. As a result, no toxic chemical solvents are needed making it a very environmentally friendly and moderately energy-intensive procedure.



The active layer strongly influences the efficiency of the solar cell. Thus, its morphology needs to be optimized and a homogenous film is desirable. In order to achieve this, spray coating is applied as deposition method for the titania/ polymer solution. It is a well-known and simple technique. One big advantage is the possibility to precisely control the thickness of the film by varying the number of spray events. Furthermore, it allows for easy mass production making it a possible method of industrialized hybrid solar cell production.

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Benchmarking the performance of thin film oxide electrocatalysts for the oxygen evolution reaction

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Oxide materials are among the state-of-the-art heterogeneous electrocatalysts for many important large-scale industrial processes, of which the O_2-evolution reaction (OER) is particularly important for energy conversion. The OER plays an important role in electrolyzers, which are key devices for the implementation of the so-called "hydrogen economy", and in particular, energy storage from renewable sources. In electrolyzers most of the overpotential comes from the side of the OER taking place on the anode, lowering the efficiency of these devices.

A specific problem arising in the study of these catalysts is the difficulty of activity benchmarking, which is challenging in many cases, especially at high current densities that are relevant for industrial applications. Under these operating conditions, serious complications arise particularly due to (i) the formation of a non-conducting gas phase, which blocks the surface during the reactions, (ii) problems in determination of the real electroactive electrode area and (iii) the large influence of surface morphology changes, i.e., stability issues, under reaction conditions, etc.

In this work, we present an approach overcoming many of these challenges, with a focus on electrochemically formed thin-film oxide electrocatalysts[1]. The approach is based on benefits provided by the use of microelectrodes, and it gives comprehensive information about the surface roughness, catalyst activity and stability. The key advantages of the proposed method are the possibility of characterization of the whole microelectrode surface by means of atomic force microscopy (Figure 1) and an accurate assessment of the specific activity and stability of the catalyst, even at very high current densities (Figure 2). We used electrochemically deposited CoO_x thin films formed on Pt-microelectrodes as model catalysts.

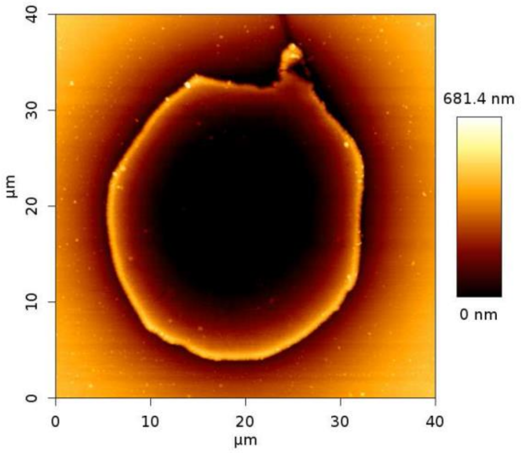

Figure 1: 2D AFM image of a deposited CoO_x layer of the modified microelectrode surface. Microelectrodes allow the characterization of the entire electrode surface.

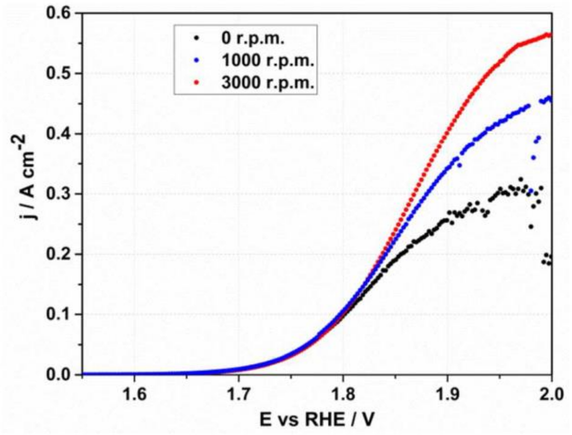

Figure 2: Rotating microelectrode voltammograms for CoO_x films in O_2-saturated 0.1 M KOH solution with and without microelectrode rotations. Potential scan rate: 1 mV/s).

1. A. Ganassin, A. Maljusch, V. Colic, L. Spanier, K. Brandl. W. Schuhmann, A.S. Bandarenka, ACS Cat., In Print, 2016. DOI: 10.1039/C5CP08000B

Material sensitive grazing incidence small angle x-ray scattering

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In recent years the use of x-rays for the investigation of the morphology of polymeric thin films in photovoltaics has increased significantly. This is due to the fact that in organic photovoltaics the performance is closely linked to the nanostructure within the thin films. X-rays can penetrate the full film and are therefore a particularly suitable tool to investigate the inner morphology of thin films. Most often hard x-rays around 8 keV are used to probe such thin films in grazing incidence geometry, namely Grazing Incidence Small Angle X-ray Scattering (GISAXS). For these short wavelengths differences in the electron density give rise to scattering. The observed scattering pattern can be used to learn about the sizes, shapes and distribution of structures within the thin films.

GISAXS is very powerful if additional information is known about the system from atomic force microscopy, electron microscopy or other complementary characterization techniques. However, in some cases it can be difficult to access the necessary information to clarify the origin of scattering contrast. Therefore, we propose a method to combine the structural analysis GISAXS with the material sensitivity of spectroscopy. Instead of using a single X-ray energy, we use resonances of particular atoms of the examined material system to gain material sensitivity. At the so-called resonant energy edges there is a drastically change in the absorption as well as in the dispersion behavior of the material containing the resonant atom. These strong changes with energy cause changes in the scattering strength, making the beam sensitive to the absorbing element. This approach has been successfully applied at the Carbon 1s absorption edge, an atom present in almost every organic molecule. [1, 2] Exploiting the strong features in the fine structure of the scattering behavior it has been shown that it is possible to distinguish different structural components from each other and hence offering a more detailed analysis of the morphology. For atoms that are present in much lower concentrations a new approach in data analysis is required.

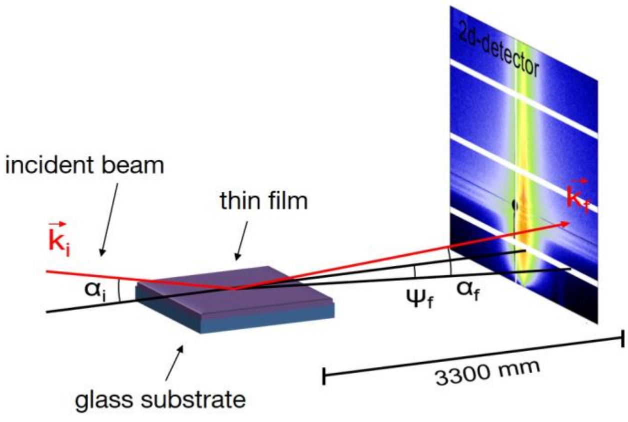

Figure 1: Schematic drawing of a GISAXS setup

Using a model system we are able to demonstrate that we can resolve the origin of scattering contrast in GISAXS measurements by varying the x-ray energy used during the experiment. In this work we will show how we obtain material sensitivity using energy dependent grazing incidence scattering experiments. Therefore, we demonstrate that the combination of grazing incidence scattering and spectroscopy is a sophisticated method for the detailed analysis of organic thin film systems.

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Modeling of the dynamic power flow in wind turbine systems with doubly-fed induction machine

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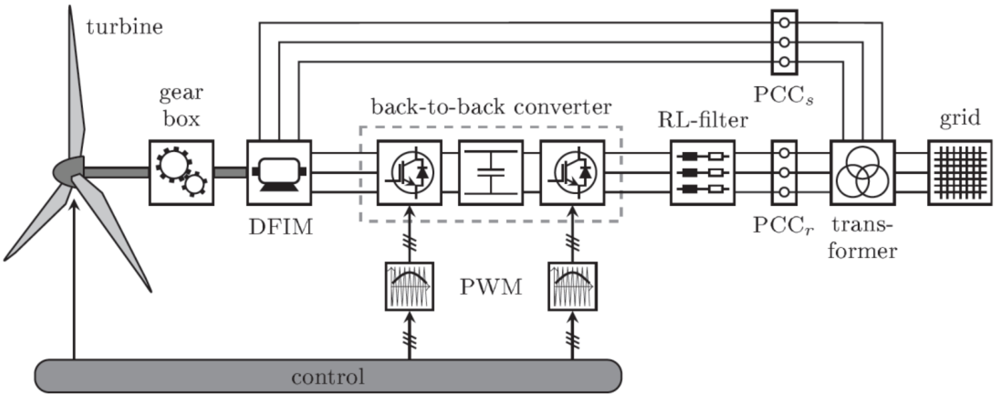

Figure 1: Wind turbine system with doubly-fed induction machine

The doubly-fed induction machine (DFIM) is one of the most common machine topologies in large-scale wind turbine systems (WTS). Around 50% of the installed onshore wind turbine systems in Germany 2013 run with this machine topology. The rising amount of wind power in the electrical power generation necessitates the knowledge of a detailed physical model of such wind turbine systems to improve the capability to meet grid code requirements and / or to participate in grid stabilization. To give better understanding of wind turbine systems with doubly-fed induction machine, the poster presents the components of which such wind turbine systems consist. By modeling the dynamical power flow within such wind turbine systems, the interaction between aerodynamical / mechanical (e.g. turbine, generator shaft) and electrical (e.g. back-to-back converter, filter) components is illustrated. The dynamic power flow allows for a detailed power efficiency analysis: An instantaneous efficiency factor can be defined as ratio between the instantaneous (active) power at the point of common coupling (PCC; injected to the power grid) and the incoming wind power at the turbine. Moreover, the poster presents two important steady state operation modes of the wind turbine systems: (i) super-synchronous and (ii) sub-synchronous operation mode.

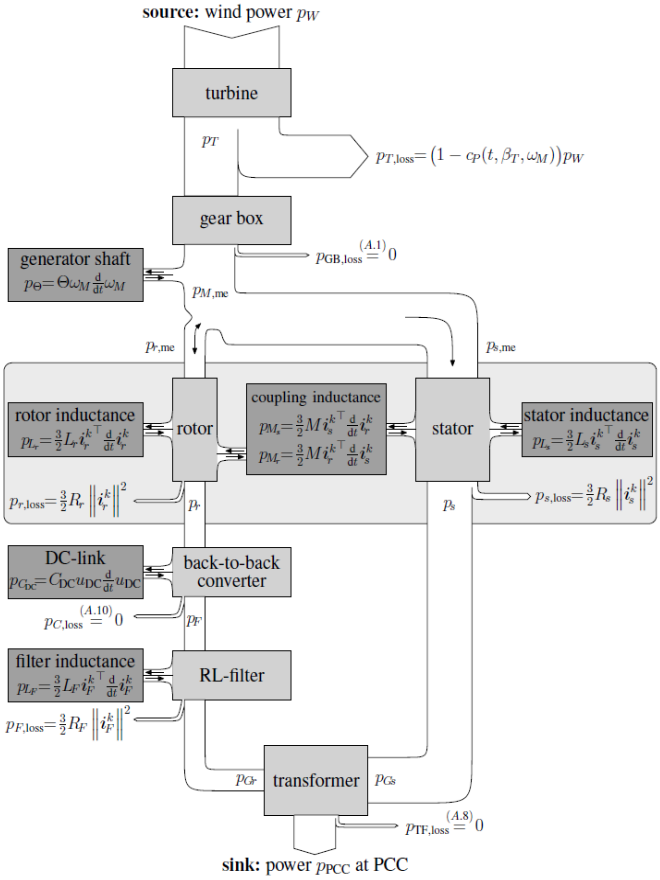

Figure 2: Dynamic power flow within wind turbine systems with doubly-fed induction machine

Thermal and life-cycle effects of timber-frame façade elements for hybrid constructions

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The research project ‘timber-frame façade elements for hybrid construction’ aims to close certain information gaps during the planning process of hybrid constructions. The project’s goal is the development of a construction catalogue, summarizing combination possibilities of highly insulated and prefabricated timber-frame elements with a reinforced concrete load-bearing structure, like skeleton or cross wall structures. This catalogue should help planners and construction companies to get standardized elements and connections. It supports the collaboration between the construction industries of timber, concrete and masonry. Though, the chairs of ‘Energy Efficient and Sustainable Design and Building’, ‘Timber Structures and Building Construction’ and ‘Concrete and Masonry’ are working together to address all questions on structural behavior, building physics –including heat, moisture, sound and fire protection– and life cycle analysis.

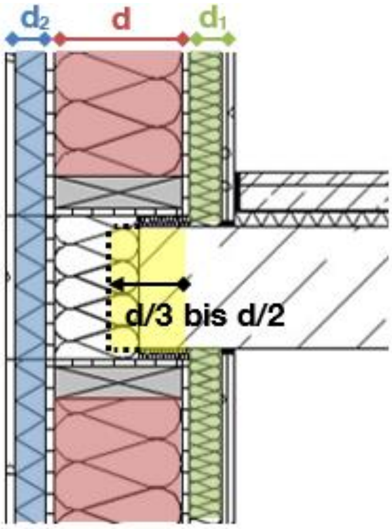

Figure 1: Connection detail wall-roof and its parameters

For example, a parametric study was conducted in order to assess the effects of thermal bridges depending on the bonding depth of the connection between façade elements and load-bearing structure. As a consequence, five exemplary projects and from that eleven connection variations from practice were chosen. The project group has analyzed the connection details regarding roof-wall, wall-floor and wall-bottom plate. Figure 1 shows the exemplary detail of a wall-floor connection. For the parametric study the timber-frame façade element is connected in different positions to the reinforced concrete structure: from one third (d/3) to one half (d/2) of the thickness of the wall’s central element (d).

The measured results demonstrate that this bonding depth (from 33 to 50 %) has a high impact on the thermal bridge coefficient ψ_e. Keeping the same u-value (0,12 W/(m²K)) and in combination with an exterior insulation finishing system (EIFS) (d_2) as well as an installation layer (d_1), the thermal bridge coefficient ψ_e changes from 0,053 W/(mK) (d/3) to 0,068 W/(mK) (d/2) – a degradation of 28 %. Keeping the same u-value and leaving out the EIFS, a degradation of about 38 % can be observed (see Figure 2). In combination with a high bonding depth of the façade elements EIFS are needed to reduce the thermal bridge influence.

Furthermore, life cycle analyses showed, that timber-frame facade elements have a positive influence on carbon footprint and primary energy demand. An example, comparing two residential buildings with the same geometry and structure but different building skins, showed that the building skin consumes 6% less nonrenewable primary energy and has 9 % less of the carbon footprint of a masonry wall for its construction and end of life. Considering the skin and building structure this translates to a 13% and 7% saving respectively. Looking at the operation phase of the building, timber-frame elements can have another significant influence: they have a much better insulation value than masonry or concrete walls for the same wall depth. Thereby, they reduce heating demand compared to buildings with same floor area and concrete or masonry walls, hence offering the possibility of increased comfort and a smaller carbon footprint.

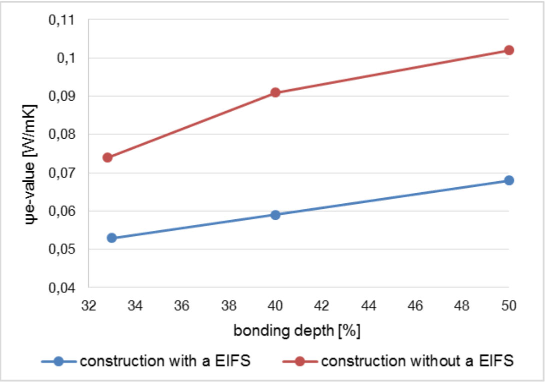

Figure 2: Thermal bridge coefficient depending on the bonding depth and construction type

Effect of magnetic field on the performance of P3HT:PCBM organic solar cells modified with Fe_3O_4 nanoparticles

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Among the different photoactive systems studied in organic solar cells (OSCs), the combination of P3HT:PCBM has been most prominent due to easy chemical synthesis and, thus, commercial availability. Regarding further increase in device performance, doping with metallic nanoparticles (NPs) has shown interesting behavior. In the case of superparamagnetic NPs, the magnetic field magnetizes the NPs, which in turn create an inhomogeneous magnetic field at the nanoscale size. Therefore, the Larmor precession frequencies of the spins of the exciton differ, which lead to intersystem crossing due to spin rephrasing. This induces an increased average population of triplet excitons, thereby extending the average exciton lifetime and, thus, lowering the recombination rate.

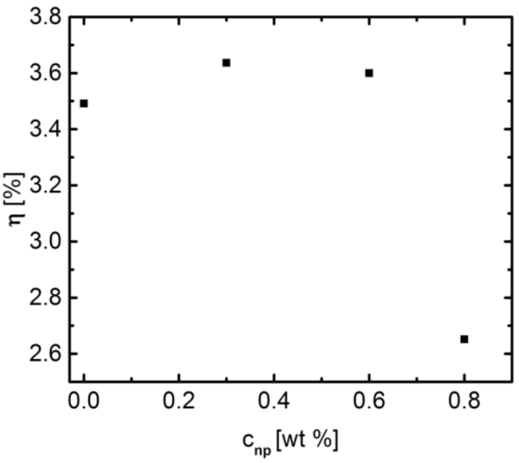

Figure 1: **PCE for P3HT:PCBM solar cells containing different weight percentages**

The aim of the present investigation is to characterize how the magnetic field and the Fe_3O_4 nanoparticles affect the performance of P3HT:PCBM-based OSCs.

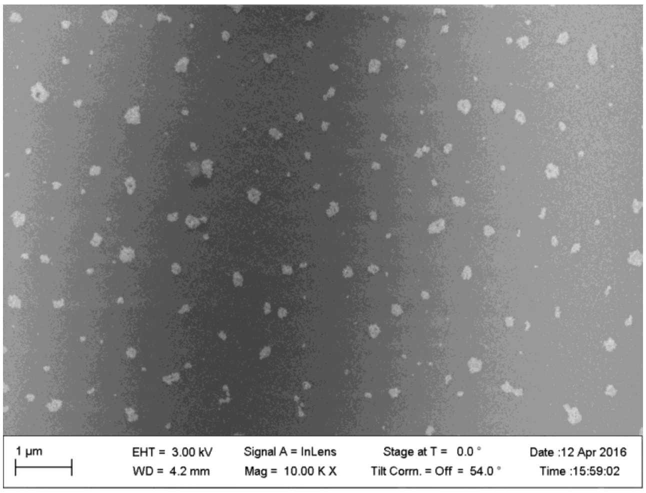

Figure 2: **SEM image of with NPs doped solar cell**

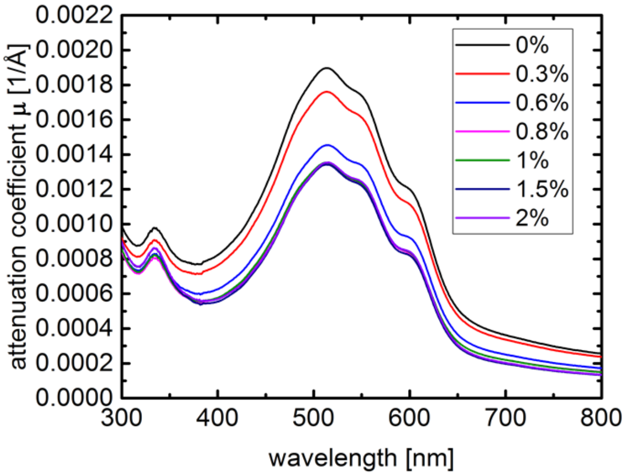

Figure 3: **attenuation coefficient for different weight percentages of NPs**

The photovoltaic performance is investigated by recording I-V curves and of the solar cells blended with different weight concentrations of iron oxide nanoparticles for different magnetic fields. The morphology is probed with SEM, AFM and scattering techniques. UVvis spectroscopy and photoluminescence measurements complement these morphology studies. Finally impedance spectroscopy, decay- and quantum efficiency measurements complete the characterization of the organic solar cells.

Explicitly Implicit Solutions:
Cavity optimization on the cheap

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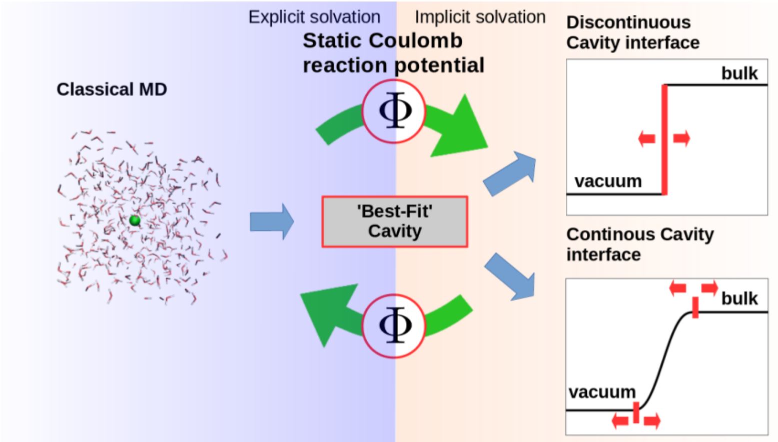

Figure 1: Schematic coupling of explicit and implicit solvation

In recent years the importance of the solvent response in catalytic, bio- and photochemical processes has become more and more apparent. Yet, in ab initio computer simulations treating the solvent effect in an efficient but accurate manner is still a major challenge.

Unfortunately, an explicit inclusion of solvent molecules significantly increases the associated computational costs. Therefore, continuum solvation models which treat the solute-solvent interaction implicitly through their dielectric permittivities, are often the method of choice. The transitions between these explicit and implicit spatial regimes define a dielectric ’cavity’ that is generally defined over a free parameter.

In our contribution, we study the validity of such an approach by comparing the implicit potential response of a multi-center multipole-expansion approach to that of explicit classical MD simulations.
We reverse engineer an optimal cavity by minimizing the differences between explicit and implicit spatially resolved electrostatic reaction potential of the solvent. To this end we also investigate a number of different models of the permittivity transition function and cavity in comparison to a modified Poisson-Boltzmann solvation approach.
Finally, we present optimization results for ions and small molecules in water.

Explicit Coulomb reaction potential

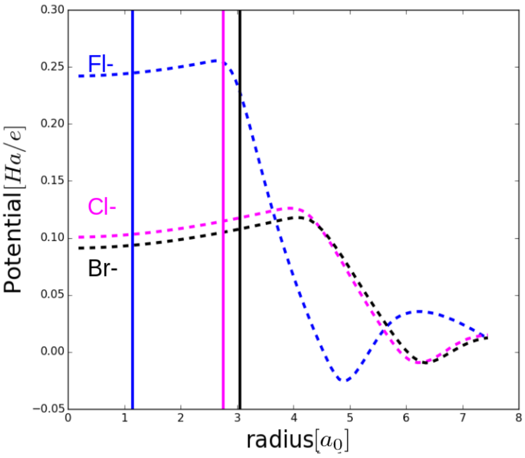

Figure 2: Reaction potentials for ions in water

Determination of the efficiency of polymer-based solar thermal collectors

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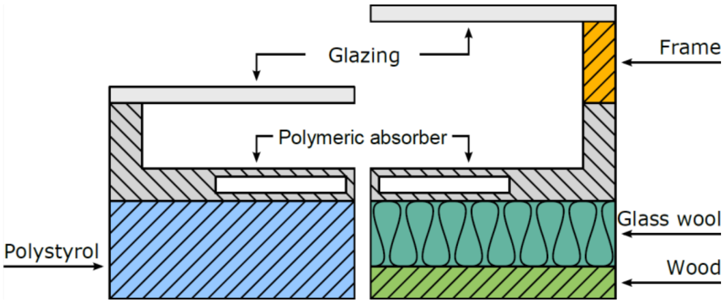

Figure 1: Setup of the colletor prototypes

Currently, solar thermal systems are facing two problems: On the one hand, declining commodity prices cause longer payback periods, on the other hand, falling prices for PV systems are a further challenge. In order to remain competitive compared to other heat generation systems, prices for solar thermal systems have to be further lowered. Cost reduction can be realized by utilizing polymeric materials both on collector and system level.

In this study we investigated to efficiency of several solar thermal collectors based on polymeric absorbers, which were provided by our project partner *Fa. Roth Werke GmbH*. In order to increase the heat transfer between the absorber and the heat transfer fluid, the risers of the absorbers are designed as rectangular channels. The absorber consists of 8 riser channels and 2 headers and has an aperture area of 0.6 m². To minimize the heat losses towards the backside, both an insulation of polystyrol and a combination of glas wool and wood has been tested (Figure 1). Furthermore, we investigated the influence of both a glas- and a PMMA-glazing (glass $\tau_{Glas} = 0.90$, PMMA $\tau_{PMMA} = 0.92$) on the solar thermal collector efficiency. As a further parameter, the effect of increasing the distance between glazing and absorber has been studied.

The collector efficiency of the prototypes mentioned above has been measured according to EN ISO 9806. Here, the heat transfer fluid gets pumped (1) through the tested collector (2). The absorbed heat gets dissipated by a heat exchanger (3) to ensure uniform collector inlet temperatures. The mass flow rate is monitored by a magnetic-inductive flow meter. An additional reservoir (5) compensates pressure changes during the test. Temperature sensors record the inlet- (6), outlet- (7) and ambient (8) temperature. Furthermore, the irradiation in the collector plane is monitored with a pyranometer (9).

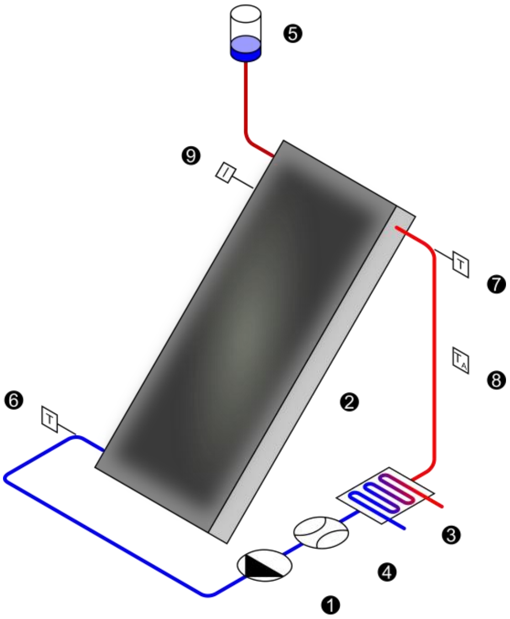

Figure 2: Test rig

The results indicate a positive influence of the PMMA glazing compared to the glass glazing. Furthermore, prototypes equipped with a backside insulation made of polystyrol cause higher collector efficiencies compared to variants with glass wool / wood, which is mainly due to the higher thickness of the polystrol insulation. Comparing the results with polymeric collectors already available on the market show a good correlation regarding the collector efficiency.

Lithium ion mobility in lithium phosphidosilicates - crystal structure, NMR spectroscopy and impedance spectroscopy of new phases in the Li-Si-P system

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There is an enhanced interest on the investigation of lithium-containing compounds due to the need for improvement of electrodes and Li ion conducting materials for rechargeable all-solid state batteries. The investigation of the ternary system Li-Si-P reveals a series of new compounds of which Li_8SiP_4[1], Li_2SiP_2[1], Li_5SiP_3, $Li_3Si_3P_7$ and $LiSi_2P_3$ are reported here.

Li_8SiP_4 and Li_2SiP_2 represent members of a new family of Li ion conductors. The Li ion conductivity ranges from 1.15(7) × 10^{-6} S/cm at 0 °C to 1.2(2) × 10^{-4} S/cm at 75 °C in the case of Li_8SiP_4 and from 6.1(7) × 10^{-8} S/cm at 0 °C to 6(1) × 10^{-6} S/cm at 75 °C in the case of Li_2SiP_2, as determined by impedance spectroscopy. Furthermore, temperature dependent solid-state ^{7}Li-NMR spectroscopy reveals activation energies as low as ~34 kJ/mol and ~46 kJ/mol for Li_8SiP_4 and Li_2SiP_2, respectively.[1]

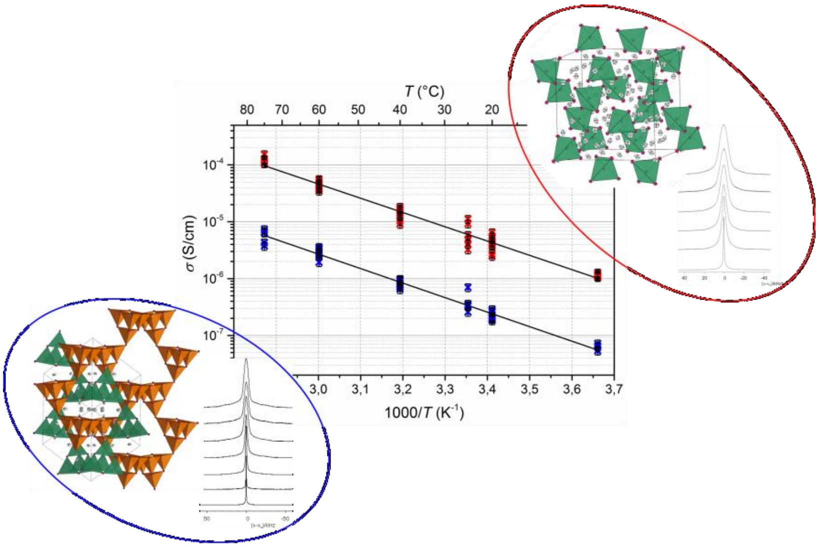

Figure 1: Temperature dependent Li ion conductivity (Arrhenius) determined by impedance spectroscopy, temperature dependence of ^{7}Li-NMR signal and structure of Li_8SiP_4 (red) and Li_2SiP_2 (blue).[1]

All compounds are structurally characterized by X-ray diffraction methods and consist of SiP_4 tetrahedra and Li ions. Li_8SiP_4 entails isolated SiP_4 units surrounded by Li atoms and reveals partially filled octahedral voids, which hint for a small phase width and ion migration pathways.[1] Li_2SiP_2 comprises a three-dimensional network based on corner sharing SiP_4 tetrahedra, where Li ions are located in cavities and channels.[1] Li_5SiP_3 contains Si_2P_6 units, which are composed of two edge sharing SiP_4 tetrahedra, $Li_3Si_3P_7$ consists of layers of SiP_4 tetrahedra separated by Li ions, while $LiSi_2P_3$ forms a three dimensional network of corner sharing SiP_4 tetrahedra with small channels filled with Li ions.

Literature:

[1] Lorenzo Toffoletti, Holger Kirchhain, Johannes Landesfeind, Wilhelm Klein, Leo van Wüllen, Hubert A. Gasteiger, and Thomas F. Fässler, *manuscript in preparation*, **2016**.

Smart Community Energy Management System Based on a Micro Market Model

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Energy policies are leading to a significant transformation in the electricity grid. It enabled integration of more renewables and replacement of nuclear and old fossil-fueled power plants. Consequently, it led to more generation irregularities and progressive dependence on the weather conditions, and the distributed energy sources within the grid. This transition forced better prediction development, robust control and merging energy markets to ensure the security of the supply. On the other hand, it encouraged the advancement of the demand side management (DSM) to integrate the residential consumer within the control or optimization cycle. Incorporating the DSM with the ongoing development within the ICT infrastructure and automation systems, the consumer is expected to be more actively participating within the energy grid and the markets.

Home Energy management systems (HEMS) are representing the doorway linking automation, ICT infrastructure and DSM within the same circle. Within a household, the HEMS represents an essential system to manage the in-house energy supplies, especially when a micro CHP, or a PV system is integrated. In such a case, house autonomy, and economic benefits are to be maximized. Yet, other goals could be maintained such as peak load shaving or minimizing CO_2 emissions.

HEMS can optimize maximize economic benefit within a household, yet individual household optimization doesn’t mean a global community optimization. A micro smart grid is one of the presented solutions that compromises between the households and the community optimization. Several researchers have been into the household optimization within the smart home and the global optimization within the grid. Yet, several obstacles are between the developed algorithms and its applications. The main obstacle is consumer privacy, as in the developed algorithms all the data must be fed to the smart grid EMS to reach optimization.

In this contribution, an innovative approach is presented for smart communities, in which a micro energy market is developed to enable heat and electricity trading between households. Such micro market enables coordination of multiple households, while maintaining privacy, maximizing economic benefits, autonomy, and above all maintaining balance between the supply and demand within the grid. In the institute for energy economy and application technology (IfE) different micro CHPs testbeds have been developed to enable realistic testing for such technology. Such micro market will be set in a hardware in the loop system (HiL), where multiple in-house supply generation technologies, and building models are integrated. Such HiL system enables accurate analysis on a realistic level of how different households with diverse in-house energy supply sources are interacting. Moreover, it facilitates deep investigation of the thermal and electrical energy consumption within the household and within the micro grid. Consequently, in this contribution, the micro market methodology will be presented, in addition to the testbed setup. Also, the preliminary results of such integrated system will be discussed and compared to both the theoretical and practical literature benchmarks.

Robust fault-tolerant control of the electrical drive adopted for airborne wind energy systems

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The idea of Airborne Wind Energy (AWE) is to replace the most efficient part of a conventional wind turbine, the tip of the rotor blade, by a fast flying high efficiency kite, and the rest of the structure by a tether which anchors the kite to the ground as seen in Figure 1. Adopting AWE systems allows exploiting higher wind speeds since the kite flies at higher altitudes (i.e. 100-300 m) compared to conventional wind towers (60-80 m). In addition to this, the cost invested in the installation and transportation is highly reduced. While the concept is highly promising, major academic and industrial research is still needed to achieve the performance required for industrial deployment. The goal of this PhD topic is to specify and model the whole electrical drive system for the AWE ground station shown in Figure 2 and to design, analyze and implement robust and fault-tolerant low-level control strategies. The expected electrical faults are specified in Table 1. Indeed, the whole system is coupled which means that a fault at one component would be translated implicitly on the whole control system. However, Table 1 identifies the possible faults and the AWE components which are directly affected by such faults. Based on dynamics, robustness and efficiency requirements, which are to be defined with the help of the network partners within the EU ITN H2020 AWESCO project, the optimal low-level control strategies will be selected and implemented for this application. The control strategy for the electric drive will be optimized for those reference inputs as reference torque or speed. Moreover, fault-tolerant control of the electrical system is essential to guarantee a safe operation of the AWE system.

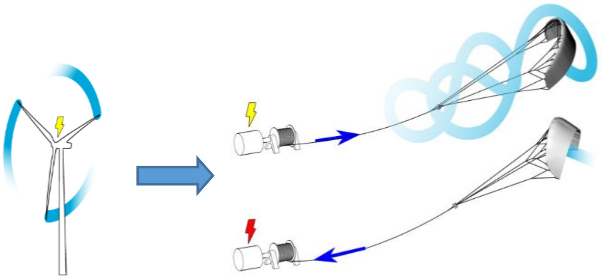

Figure 1: AWE concept compared to conventional wind turbines

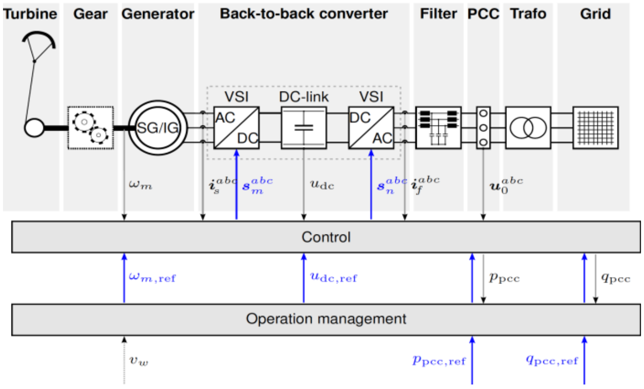

Figure 2: Typical low-level components for AWE system

Table I: Possible electrical faults and their direct correlation with the AWE components

Types of electrical faults	Permanent Magnet SG	Generator-side VSI	Grid-side VSI
Interior windings s.c	✓	-	-
Windings o.c	✓	-	-
Line-Neutral s.c	-	✓	✓
Line-Line s.c	-	✓	✓
Line-Line-Line s.c	-	✓	✓
DC link s.c	-	✓	✓
Loss of DC link voltage	-	✓	✓
IGBT failure	-	✓	✓
Grid voltage sag/swell	-	-	✓

s.c: Short circuit, o.c: Open circuit

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Fabrication and characterization of hybrid organic-inorganic perovskite films for solar cell applications

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Electricity is needed in many situations of our daily life at many different locations around the globe and in space. Naturally, it has been a longstanding scientific quest to find different possibilities to convert energy present in our environment to electricity. Solar energy, although not available 24/7, has the major advantage that the “fuel” for the conversion process is simply available during daylight. It does not have to be actively transported or stored and is free of political control. Therefore, a strong interest in solar energy conversion has manifested over the last decades with solar cells taking the role of converting solar energy to electricity.

The desire to efficiently convert solar into electric energy has led to increasing activity in the associated field of scientific research in the last decades. In 2015 38.000 GWh, i.e. around 20% of the renewable energy consumed within Germany was obtained from photovoltaic installations [1]. To further increase these numbers and to exploit advances in material science, novel, high performing solar cells are strongly sought after. A new strand of solar cells currently focuses on exploiting solution processability together with major advantages, such as low material costs, low weight and mechanical flexibility. Manufacturing solar cells from solution promises significant cost reduction, however, while much progress has been made disadvantages such as comparatively low efficiency inhibit mass production so far.

While most of the progress has focused on so called organic solar cells, where organic, mainly polymeric compounds are used for the light converting layer, the recently discovered ability of perovskite materials to act as highly efficient light conversion layers has led to a strong shift of research direction. Combining advantages of organic and inorganic systems, perovskite solar cells - as hybrid organic-inorganic cells - have shown a steep rise in efficiency over the last few years, already having reached a little more than 20 % in lab scale devices. It has been found that the crystal structure of perovskite cells is of utmost importance for its performance. Therefore, it is highly desirable to understand under which conditions the relevant structures form and which cases they do not.

In our group we are able to track morphological changes during the preparation of active thin films and can even do so under different environmental conditions. Our collaboration partners at the NTU, Singapore, have strong expertise in the preparation of high performance perovskite solar cells. Together we have formed a project to combine our expertises to resolve structure formation processes in perovskite thin films for the application in solar cells. These results will deliver key elements for the understanding of how to further improve this type of solar cells.

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[2] A. Sharenko, M. F. Toney, Journal of the American Chemical Society 2015, 138, 463.

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Multi-Objective Optimization and Coupling of Passive and HVAC systems to Enhance the Integrated Performance of Office Building Façade

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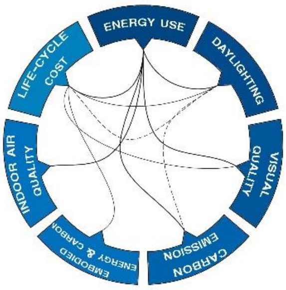
Building facades have great impact on the buildings energy consumption and users' comfort. The facades must achieve different functions while maintaining the energy consumption of the building as low as possible. As some of these functions might conflict with each other, architects and designers usually use a trade-off approach when designing high performance buildings facades. Nevertheless, due to the numerous aspects affecting the overall building performance and the mutual effects between these aspects, the complexity of an integrated design approach increases significantly. Therefore, integrating performance simulation and optimization tools becomes a necessity.



The complicated relations between the different environmental aspects requires a more coherent and integrated approach.

Figure 1: Environmental performance aspects of building's facade

The focus of this paper is devoted to the notion of complex adaptive systems. Building facades perfectly lies within the general definition of complex systems as systems consisting of large numbers of relatively simple, autonomous, yet interconnected elements. Using complex systems based approach proves to have a great potential in binding currently separate developments of building technology and theory into an open, creative and highly efficient architectural system.

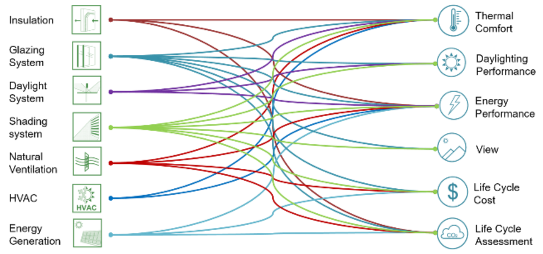


Figure 2: Holistic approach for facade performance

Several previous research work had focused on enhancing the building's form through the aid of environmental simulation tools as well as optimization tools. However, on most cases they were mostly limited to single optimization criteria (minimizing energy use, solar exposure, daylighting, etc.) or specific building system (façade construction, glazing system, HVAC, etc.). It could prove to be more beneficial to deal with building facades as a complex adaptive system. Accordingly, this research is extended in considering more aspects while utilizing the multi-objective trade-off approach to arrive at several different optimal façade designs.

The main aim of this paper is to examine the effectiveness of using multidimensional optimization for optimizing the integrated performance of buildings' façade with respect to the total energy consumption, daylight quality and thermal comfort. A special focus was given to the effect of coupling both passive design techniques (solar shading, façade building construction and high performance glazing) and the HVAC system elements. The optimization variables tested are: the window-to-wall ratio (WWR), Glazing type, insulation thickness, sun shadings and daylighting systems, and the HVAC elements.

A parametric model of a single office space was created using Grasshopper plugin for the Rhino 3D CAD software. The effect of changing the variables on daylighting performance was measured using Radiance simulation engine. Additionally, Energy Plus software was used to model the HVAC system and calculate the total Energy Use Intensity for the office zone, as well as to measure the effect of changing the model variables on the thermal comfort for the occupants. A multi-objective optimization was used afterwards in order to reach an optimal range of solutions (Pareto front).

Synthetic strategies to mesoporous undoped and phosphorus doped germanium morphologies with inverse opal structure as anodes in lithium ion batteries

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Silicon and germanium are of great interest as anode materials for lithium ion batteries due to their large theoretical energy densities. Germanium is less abundant but stands out due to its two orders of magnitude higher lithium ion diffusivity and four orders of magnitude higher electronic conductivity than silicon.[1] By the introduction of dopants the electrochemical properties can be further optimized. We previously established a combined dip-coating/drop-casting technique to obtain inverse opal structured germanium thin films on a wide variety of substrates (copper, silicon, silica, sapphire, FTO, ITO) which may also allow for phosphorus doping.[2]

Herein we report various synthetic strategies (e.g. spin-coating, spray-coating) to up-scale the received ordered germanium networks and we investigate the possibilities of phosphorus doping.

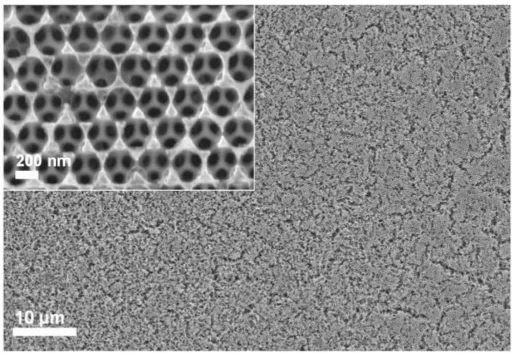

Figure 1: SEM micrograph of an obtained Ge film.

Based on the controlled oxidative decomposition of Zintl clusters in presence of a template structure we utilized several different coating techniques to prepare homogenous germanium thin films with inverse opal structure. Concretely, we succeeded to prepare and dope germanium films with adjustable pore size assembled from K_4Ge_9 Zintl clusters using a wet-chemical method. Red phosphorus, tripenylphosphine or sodium heptaphosphide were used as P sources for phosphorus doping.

Morphological analysis of the obtained films by scanning electron microscopy (SEM) displays the formation of ordered mesoporous networks with adjustable pore size, depending on the template. XPS studies were performed to investigate the influence of various P sources. Electrochemical studies show promising results concerning long term stability and coulombic efficiency.

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Ge_9- and $Ge_{9-x}Si_x$-ZINTL Clusters as Wet Chemical Precursors for Mesoporous Ge- and $Ge_{1-x}Si_x$-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] Especially, ordered porous inorganic semiconductors are promising for application in those solar cells, but the routes to periodic porous materials are scarce.[2] Particularly, bottom-up approaches based on directed self-assembly of molecular precursors are desirable, due to an unprecedented control over the shape, size and spatial arrangement of the pores.

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 pore size of approximately 300 nm using solutions of the intermetallic compound K_4Ge_9 which contains nine-atomic clusters.[3]

Herein we present the controlled coupling of Si-Ge mixed ZINTL clusters starting with less soluble phases $K_{12}Si_xGe_{17-x}$ for the bottom-up fabrication of periodic porous silicon-germanium morphologies.

The results on the $Ge_{1-x}Si_x$-films are compared to the pure Ge films by means of morphological and electronical analysis using Scanning Electron Microscopy (SEM), Raman and X-Ray Photoelectron Spectroscopy (XPS).

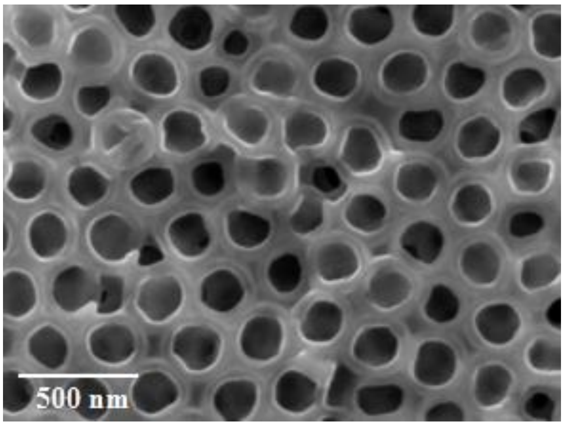

Figure 1. SEM of inverse opal structured Ge/Si

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Tungsten fibre-reinforced tungsten composites – Development of a high temperature material for fusion application

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Tungsten is a promising candidate for the use as a plasma facing component in a future fusion device due to its (unique properties such as a) low sputter yield, high melting point and moderate activation. The brittle behavior of tungsten below the ductile-to-brittle transition temperature and the embrittlement during operation e.g. by overheating and/or neutron irradiation are the main drawbacks for the use of pure tungsten. This limitation is mitigated by using tungsten fibre-reinforced tungsten composites (WfW) which utilizes extrinsic mechanisms to improve the toughness similar to ceramic fibre-reinforced ceramics. It has been shown that this idea in principle works in as-fabricated state as well as after embrittlement. The material shows enhanced performance in bending tests, charpy impact tests and tensile tests.

The next step is the conceptual proof for the applicability in fusion reactors. This will be done by producing mock-ups and testing them in cyclic high heat load tests. For this step the material needs to be further developed and all constituents of the composite, which are fibre, matrix and interface, and all process steps need to be addressed. In this contribution we will exemplarily present studies on new interface systems and here in particular recent results on titanium nitride (TiN).

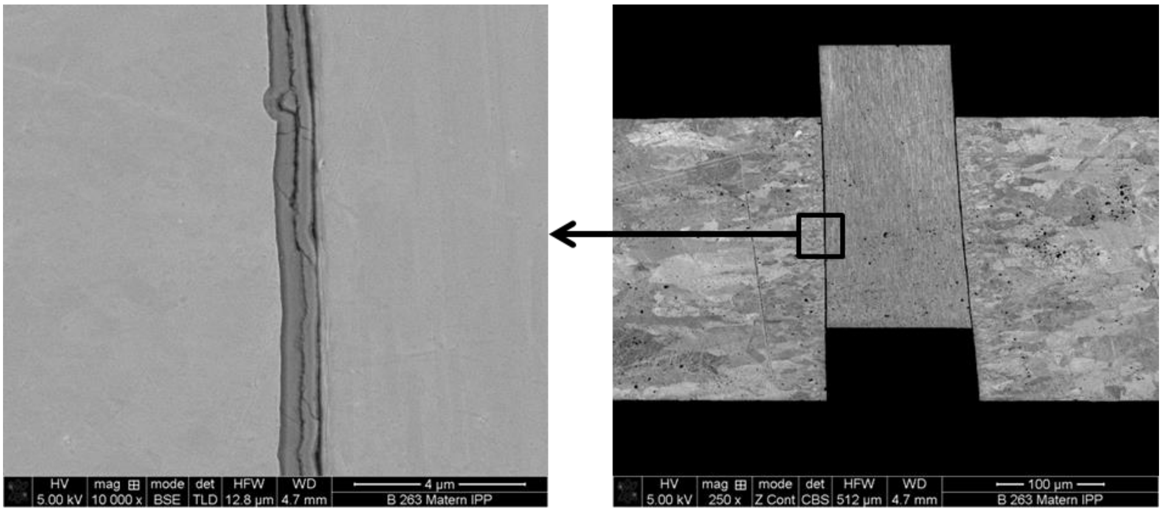

Figure 1: TiN as an interface Material after a Push Out test

The interface material plays a crucial role in the behavior of the composite material. The interface material and the bonding of the materials have to be weaker than the fibre and the surrounding matrix, but the material has to be strong enough to bear load and transfer the stresses from the matrix to the fibre.

New interface systems have been studied in respect to their applicability in WfW by means of push-out tests on single fibre model systems. A single fibre is coated by a PVD process and embedded into a tungsten matrix. Push-out tests are used to evaluate the interface strength and the failure mechanisms. The investigation is supplemented by a detailed microstructural investigation before and after the mechanical tests.

Thermal Conductivity of Thin Films Determined via IR thermography

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In fields such as microelectronics and thermoelectrics, heat management becomes increasingly important. With the continuous miniaturization of the corresponding devices, established methods such as direct on-chip thermal conductivity measurements, the Raman-shift method, or thermoreflectance characterization face severe challenges. Among them are the influence of the substrate, long measurement times, complex calibration processes, and difficulties when applying these methods to porous films. To overcome these challenges, we propose and realize a novel and simple method for the measurement of the in-plane thermal conductance of thin films using infrared (IR) thermography.

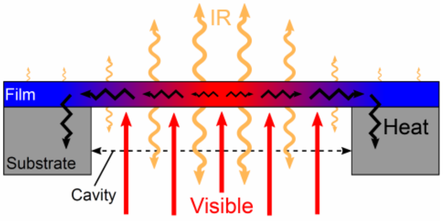

Figure 1: Schematic sketch of the infrared thermography method developed.

In order to measure the thermal conductance a temperature gradient has to be introduced. A possible measurement geometry for this in conjunction with IR microscopy is shown in Fig. 1. Here the thin film to be characterized is suspended above a round cavity in an otherwise opaque substrate and is illuminated by a laterally homogeneous light source from below. The light is absorbed by the thin film and heats it while the substrate acts as a heat sink. For this geometry an analytical solution for the resulting temperature distribution can be found. The paraboloid that describes this distribution depends only on the film thickness, the absorbed power density, and the sought-after thermal conductivity. In order to measure the temperature distribution, a contact free method is preferred, such as via infrared microscopy, which in particular allows the single-shot capture of full two-dimensional temperature profiles. This is realized by placing a suitable IR microscope above the film. The necessary calibration of the microscope is done on the sample with a heater and a thermocouple.

Here we apply this versatile and quick method to the thermal characterization of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) and polyimide. Figure 2 a) shows an IR image of such a PEDOT:PSS film suspended over a hole, visible as a grey circle. Outside of the circle the surface of the aluminum substrate can be seen underneath the film. When the film is illuminated by the LED light source, it heats up, appearing brighter in Figure 2 b). Figure 2 c) shows a false color image of the resulting temperature distribution after calibration was applied. An area of roughly 10x10 mm^2 is captured with one image, showing that a large sample area with several holes can be studied simultaneously, providing ample amounts of data for a statistically relevant analysis. While there is hardly any temperature change for the film covering the aluminum, evident by the black color, the suspended film shows a significant increase in temperature under optical heating, shown by the bright coloring. The data acquired can be fitted well with the paraboloid introduced above as shown in Figure 2 d). The thermal conductivities of 1.0 and 0.4 W/(mK), acquired for PEDOT:PSS and polyimide, respectively, are in good agreement with literature values. These proof-of-principle experiments demonstrate the validity of the new technique and will now be extended to systematically investigate the influence on the thermal properties by varying the electrical conductance and adding nanoparticles to the polymer film.

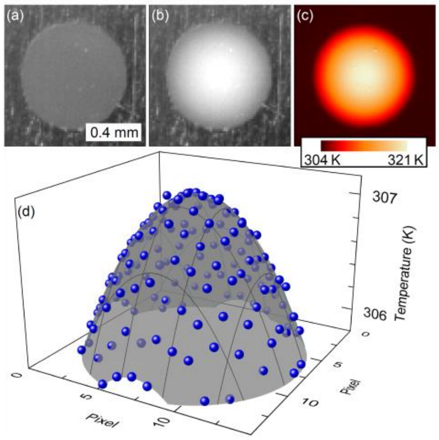

Figure 2: IR topography of suspended PEDOT:PSS a) without and b) under illumination. c) Temperature distribution under illumination. d) Exemplary fit (grey surface) of a measured temperature distribution (blue dots).

Synthesis and Characterization of Metal-(Mabiq) Complexes, and Investigation of Their Reactivity for Hydrogen Evolution

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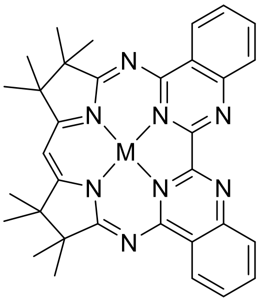
Hydrogen derived from non-carbon compounds has emerged as a potential source for sustainable energy production, which minimizes carbon dioxide emissions. Hydrogen production via water splitting (reduction) appears to be a convenient solution for the long-term storage problem of solar energy. The potential use of hydrogen as a form of renewable energy storage has prompted efforts to increase the development of new catalysts to promote its catalytic generation from acidic solutions. Complexes comprising earth-abundant transition-metals have been studied extensively as electrocatalysts. Besides cobalt and iron complexes, macrocyclic nickel complexes arise as promising systems for catalytic hydrogen evolution.[1]-[4]



Metal-(Mabiq)

Figure 1 : Structure of the Metal-Mabiq complexes

We will present results of studies with a series of new metal-complexes (nickel and cobalt), coordinated by a redox-active macrocyclic ligand (Mabiq). The formally Ni(II)- and Ni(I)-complexes as well as the Co(III), Co(II) and the Co(I) forms have been successfully isolated and structurally characterized using different spectroscopic methods, including XRD, NMR and absorption spectroscopy. Reactivity and electrochemical studies indicate activity for the newly synthesized nickel- and cobalt-Mabiq complexes with respect to catalytic hydrogen production.

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Regulating the potential for Li_2S activation by selection of electrolyte and additive in lithium-sulfur battery

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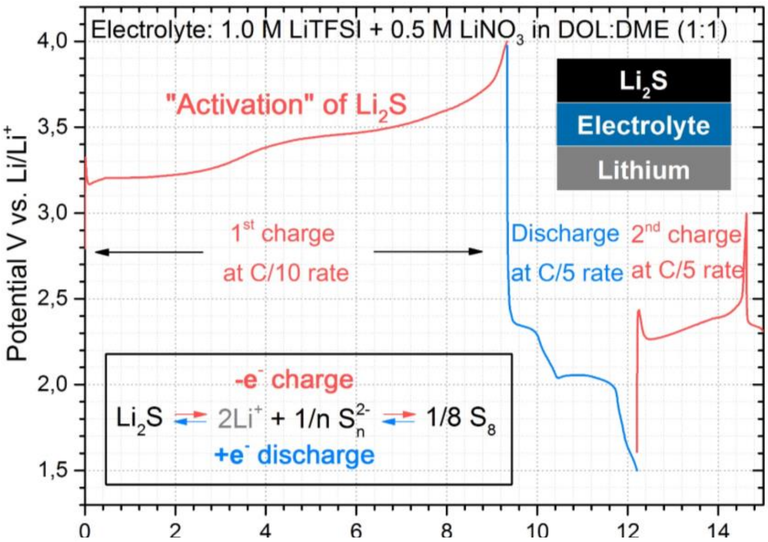

Figure. 1: Typical galvanostatic charge and discharge profile of $Li_2S//Li$ battery in a swagelok cell configuation

In the search for high energy density and inexpensive post Li-ion batteries, lithium-sulfur batteries have been intensively researched due to their high theoretical capacity (1675 mAh/g), natural abundance and non-toxicity of elemental sulfur.[1-4] However, the development of Li-S batteries has been limited due to insufficient understanding of solvent´s influence on the Li-S chemistry. For instance, it has been reported that a high potential is required to "activate" the Li_2S in the very first charge process with commonly used electrolyte (DOL:DME) in a $Li_2S//Li$ battery system (fig.1),[2-4] although in other electrolyte system, e.g. DMA, a significant lower potential has been shown for this activation process.[2,3] These studies, however, did not clearly reveal which property of solvent/additive is relevant for this activation process and its mechanism remains still unresolved. Therefore, in this work, we try to understand the dependency of this activation process (1st charging process of Li_2S) on solvent´s property in a $Li_2S//Li$ battery system.

Our recent work (will be shown in the poster), shows that the donor number of the solvent may play a relevant role in the reduction process of Li-S system and we hypothesize that the degree of lithium ion solvation affected by the donor number of the solvent leads to different degree of polysulfide (S_n^{2-}) stabilization, which in turn alters the Li-S reduction process.

Combining this finding and our new understanding of the Li_2S charging mechanism,[4] we propose that the donor number of solvent could also play a critical role for Li_2S activation in the 1st charging process. To verify this hypothesis, we selected several solvents with various donor numbers and examine their performance in galvanolstatic cell charging using conventional Swagelok-type battery cells and in-house designed two-compartment cells, which enables us to use different electrolyte in the cathode compartment and in the anode compartment.[2] To further understand and confirm our hypothesis, several additives, which could affect lithium ion solvation or can interact with polysulfide intermediates, are also investigated.

Acknowledgement

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Methods for Identifying, Analysing and Influencing Material Flows in Urban Areas – A Contribution to Resource Management in the Building Industry

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According to estimates of the German Federal Ministry for the Environment, the German building stock contains around 10.5 billion tonnes of mineral building materials, around 220 million tonnes of timber products and around 100 million tonnes of metals. Due to continuous building activities, especially renovation and retrofit measures, it is estimated that this raw material stock will grow by a further 20% until 2050 [1]. The building sector is one of the most resource intensive economic sectors in Germany. The German National Strategy for Sustainable Development sets targets of doubling the raw material productivity until 2020 based on 1994 levels [2]. The developed raw material flow model for the building industry that is described within this abstract can aid in reaching these proposed targets.

The major aim of this project is to analyse the construction related material flows over the whole life cycle of urban areas. The basis for this inventory sets the identification of what types of materials and how much are contained in different building types of the German building stock and selected infrastructure such as roads. Furthermore, a developed life cycle model can give an indication at what times raw materials are required (e.g. insulation for retrofit, or new construction), and when raw materials and potential pollutants become available again, for recycling or disposal, after the end of life of individual components of the analysed area.

The developed raw material cadastre can then be integrated into geographic information systems (GIS), such as the CityGML standard as an additional layer and be linked to energy information for example (e.g. heating demand), to analyse the influence of raw material flows on the energy consumption of individual buildings and the analysed area as a whole. As the individual material flows (life cycle inventory) will be identified, it will also be possible to link this information to life cycle assessment (LCA) data to identify the environmental impacts (e.g. CO_2 emissions) the continuous changes of urban systems and the anthropogenic stock may have.

This integrated approach is not only examining the life cycle of material flows of urban systems over time, but it also tries to link and provide an interface to existing systems and calculation methods, to move towards rating the overall resource efficiency over time. As stated in VDI 4800, a conclusive rating of the overall resource efficiency of systems can only be achieved if the use of all natural resources is being quantified and then placed into relation with each other [3].

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Towards a CO$_2$-neutral TUM Campus Challenges & Opportunities

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With a total electricity and heat demand as high as 85 GWh/a resp. 75 GWh/a and an equally high cooling demand of 13 GWh/a combined with an own power plant and heating and electricity grid, the TUM Campus in Garching presents an ideal test bed to implement the 'Energiewende' and assess the impact of the currently much discussed 'sector coupling' on-site. Based on a simultaneous simulation of the electricity, heat and cooling demand and supply system, this talk explores different routes towards a CO$_2$-neutral campus. Possible future scenarios along with the various strategic options and challenges will be outlined and put up for public discussion.

With 12,000 students and 6,000 employees, the TUM Campus Garching is currently already one of Germany's largest university facilities. In the next years, a significant expansion of the campus is planned, requiring a further development of the current energy supply system. Core of the current system (shown in figure 1) is a 4 MW$_e$ and 6.5 MW$_{th}$ Cheng Cycle, a flexible and innovative gas turbine cogeneration plant. Together with 2 gas boilers, the Cheng Cycle covers 100 % of the heat demand and 40 to 50 % of the electricity demand on-site. Cooling is currently provided by a combination of compression chillers, absorption chillers and numerous split air-condition units. The high consumption combined with a local management and a medium voltage electricity grid is representative for industrial and commercial sites.

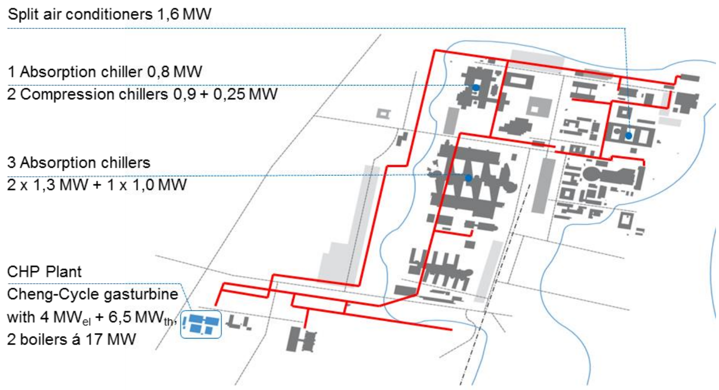

Figure 1: Energy supply Campus Garching

To increase the share of renewable energy and improve the overall efficiency of the energy system, a mix of promising future technologies is assessed and possible perspectives for the energy supply system are identified.
Considered technologies are for example fuel cell cogeneration plants, biomass gasification, organic Rankine cycles as well as storage systems such as power-to-gas and thermal storage. Besides heat and power generation, the optimal cold supply system is also investigated. To this end, both compression and state-of-the-art absorption chillers are considered.

To describe the power system, the energy system model URBS is used. URBS is a linear programming optimization model for capacity expansion planning and unit commitment for energy systems. The model consists of a linear objective function that represents the annual total costs for the energy system under investigation. The technical and economic properties of all system components are modelled with linear inequality and equality constraints. The decision variables capture size and operation of all energy conversion technologies under consideration.

The results show promising supply systems for the campus in Garching, each with the resulting overall costs. With different scenarios different objectives are satisfied. These are for example the reduction of the current CO$_2$ emissions by at least 40 % up to 80 %, the reduction of the consumed primary energy and therefore also the increase of the overall efficiency of the energy supply system. Possible directions for the future development of the TUM campus Garching will be shown and put up for discussion, delivering a better basis for decision-making regarding future investments in the local energy supply.

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Hybrid photovoltaics based on diblock copolymer structured, mesoporous Ge thin films

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The challenge of providing sufficient energy for a growing world population with limited oil, gas and coal resources has led to increasing interest in renewable energies in the last decades. At the same time the negative impact of fossil fuel combustion on the environment gets more and more visible. Especially photovoltaics is a promising candidate for future energy provision, as the energy of sunlight reaching the earth could easily cover the world energy consumption.

In this context, hybrid photovoltaic (HPV) devices are a promising technology, which combines the advantages of conventional semiconductor-based and of organic solar cells. The semiconductor material, which acts as a framework for the active layer, provides high charge carrier mobility and enhances the chemical stability of the cell. The organic component offers cost-efficient, large scale production and the synthesis of flexible devices for various applications.

Combining diblock copolymer templating with sol-gel synthesis of an inorganic precursor is a sophisticated method to produce the mesoporous, inorganic part of the active layer. The micellar solution of the diblock copolymer and the precursor particles is deposited on a substrate via spin coating. After removing the diblock copolymer via calcination, one can infiltrate the sponge-like structure with the organic hole-conductor. This bottom-up approach has the advantage of precise control over the morphology. Especially porosity and pore size are of crucial importance, as a large interface between the two materials as well as percolation paths have to be ensured. Furthermore, the structure size has to be in the range of the exciton diffusion length to minimize recombination losses.

The synthesis of mesoporous structures based on titania has been demonstrated with polystyrene-block-polyethylene oxide as an amphiphilic copolymer and titanium tetraisopropoxide as a precursor [1]. Similarly, a mesoporous network of germanium can be synthesized by using Zintl clusters like K_4Ge_9 [2]. Germanium offers new possibilities in terms of band alignment as well as good electron conductivity and, therefore, could be an important alternative for HPV devices. Primary investigations comprise surface structure analysis via SEM (Fig. 1), spectroscopic absorption behavior via UV/Vis as well as crystallinity characterization via XRD.

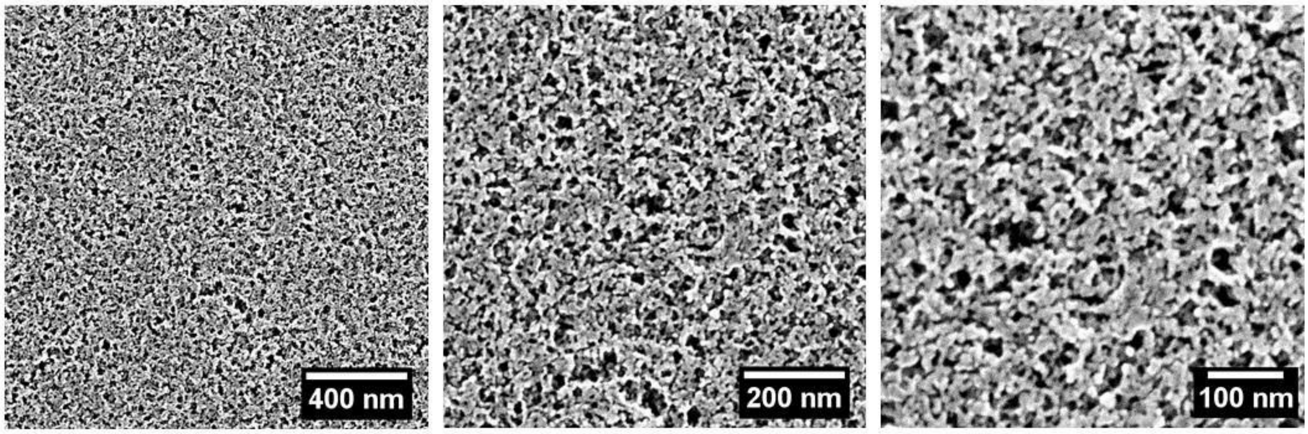

Fig. 1: SEM images of a mesoporous titania network at three different magnifications

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Effect of Reduced Rotational Inertia on Frequency Stability in the European Transmission System

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The behavior of system frequency during a mismatch between supply and demand (i.e. caused by a generation or load outage) is dependent on the operating rotational inertia of the power system, which is predominantly provided by conventional synchronous generating units. The large-scale integration of converter-interfaced renewable generation will result in a reduced role for conventional generation within the future European power system, potentially leading to significant reductions in operating rotational inertia. Under critical conditions, such as at times of low demand during which the amount of operating synchronous generation is commonly at a minimum, this reduced rotational inertia may result in large frequency deviations during power imbalances. If such deviations exceed rated disconnection settings for renewable or conventional generation, cascading failure may occur. Further, if such deviations exceed frequency settings for load-shedding actions, customers will be subjected to blackout conditions in order to prevent total system failure, as shown in Figure 1. Such scenarios represent a significant challenge to frequency stability.

The presented research examines the effect of reduced rotational inertia in the context of the future European electrical transmission system. A detailed dynamic model of the entire synchronous transmission system (380 kV and 220 kV) is developed (see Figure 2) and a range of possible developments in installed PV and wind capacities are investigated. Through simulation of large power plant outages, the influence of the installed renewable capacities on the frequency deviation is ascertained. Corrective measures are considered, such as the contribution of synthetic inertia from wind turbines.

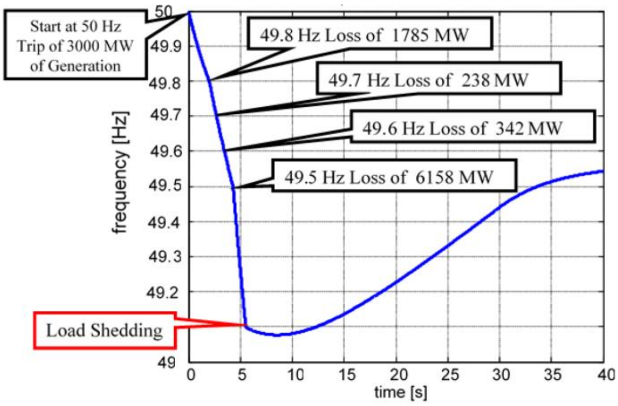

Figure 1: Frequency deviation after power plant outage [1]

Figure 2: Transmission system model

Literature:
[1] ENTSO-E, ‘Dispersed Generation Impact on Continental Europe Region Security’, Brussels, Belgium, 2014

Developing alternative material systems for energy conversion through hybrid photovoltaics

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For the past century the world energy supply was based on fossil fuels. Due to their limitation, most recent developments of the world energy supply show a transition to sustainable and renewable energy sources. Among those, photovoltaics has generated a common interest due to the immense potential of the sun's energy. According to the International Energy Agency the world's total energy consumption could be easily covered by harvesting only a small portion of the solar energy of around 10^{21} Wh reaching the earth's surface. Thus, the development of ways to harvest this abundant, clean and readily available energy form is playing an emerging role.

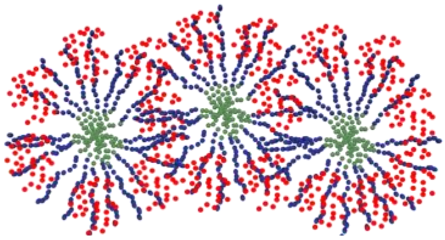

Figure 1: Diblock copolymer template for mesoporous structure synthesis

Within this frame, inorganic-organic hybrid photovoltaics (HPV) face this challenge through combination of the advantages of both organic and inorganic materials. While the inorganic part contributes high charge carrier mobility and chemical stability, the organic counterpart offers the possibility for large scale/low cost processability and flexibility. Compared to organic solar cells, structural/morphological degradation effects are less important. The inorganic material acts as a framework, which inhibits such like degradation, and enhances HPV lifetime stability.

The inorganic component of such a device must fulfill several conditions to be suitable for a HPV device. Primarily, the possibility of infiltrating the layer with the organic hole-conducting material must be assured. Therefore, precise control over the degree of porosity and pore sizes is of major importance. One promising pathway to build up such an inorganic framework consists of a polymer-templated bottom-up approach combined with sol-gel chemistry, which allows for the synthesis of high surface-to-volume ratio thin films. While the structural behavior of this routine has been broadly studied for titania thin films [1] research on alternative material systems is very limited.

On this basis, new polymer templated sol-gel routines are developed to allow for the incorporation of alternative precursors such as germanium. In addition mesoporous titania based films have been synthesized to be combined with novel organic molecules. These layers build the foundation for a vast range of new, promising possibilities of material systems for HPV applications.

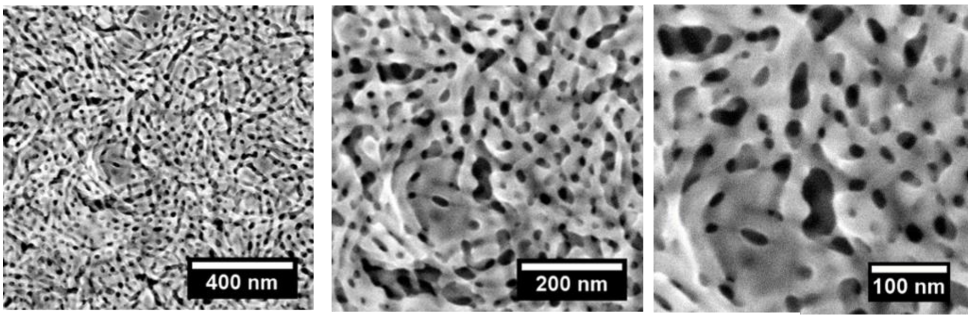

Figure 2: Mesoporous Ge layers for HPV applications

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[2] K.Sarkar, E.V.Braden, S.Pogorzalek, S.Yu, S.V.Roth, P.Müller-Buschbaum; ChemSusChem **7**, 2140-2147 (2014)

Optimisation Framework for Residential Energy Systems

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With all the changes occurring within the energy system landscape it is necessary to have a framework where various energy efficiency measures can be evaluated and compared. A residential energy system optimisation framework is presented that uses a dynamic model of one residential unit as a building block, shown in Figure 1. Both the thermal and electrical parts of the energy system are modelled, in order to evaluate the impact technologies such as Power-to-Heat as well.

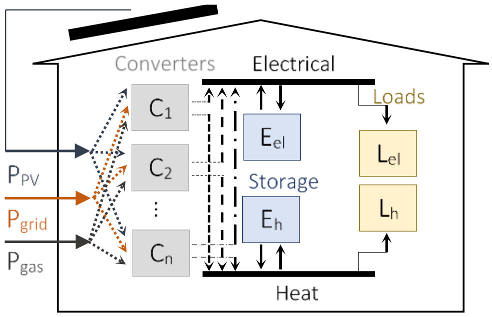

Figure 1: Residential Unit Building Block Structure

This framework is a flexible tool to study energy efficiency measures in an urban context. For example, it can be used to evaluate the Demand Side Management (DSM) potential of a heat pump with a floor heating system, by introducing flexibility into the heating load, allowing the indoor temperature to have a range. In order to optimize the operation of thermostatically controlled loads on a building to building block or city quarter level, a simplified modelling approach describing the thermal behavior of a building is chosen instead of a complex one to ensure scalability. Using a simplified single zone house model, a third order RC model is derived using thermal-electrical analogy.

A Model Predictive Control (MPC) is used to control the system, and it can be designed to consider different optimization criteria. For control of heating systems, it is useful to formulate a cost function incorporating both a term for discomfort and energy consumption, where discomfort is the variation of indoor temperature from a certain set-point. The energy saving potential of the heat pump is evaluated by including a PV infeed and trying to maximize self-consumption, and the tradeoff with discomfort is also investigated.

Another interesting investigation that this framework is useful for, is the coordination between multiple residential units. For this a Distributed Model Predictive Control (DMPC) algorithm is developed. Mostly MPC is implemented in centralized schemes, however it scales badly with the size of the system, since the optimisation has to be performed for several time instances.

The aim for the DMPC is to coordinate the behaviour of several residential units to obtain synergy benefits, without having to optimise the entire system with a centralised controller. This is done by distinguishing between the Centralised Controller (CC) and the Local Controller (LC), where the former will not perform any optimisations. The DMPC framework principle is applied to a case study example, which is the coordination of four houses where one of them has PV infeed and three of them have an electrical energy storage or a heat pump.

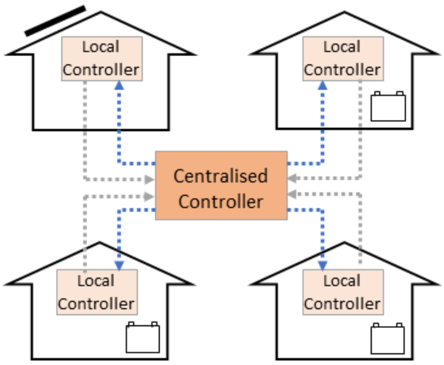

Figure 2: Control set up for DMPC

Running a three day simulation shows that the DMPC can improve self-consumption significantly, and that a centralized controller is not essential, making the optimization framework both flexible and scalable.

Morphology and conductivity of ionic liquid/block copolymer hybrid electrolytes for lithium-ion batteries

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Lithium-ion battery is one of the most popular energy storage systems, not only for electronic devices like laptops, cameras or mobile-phones, but also for electric vehicles. This is due to several advantages like high power to weight ratio, long cycle lifetime and low self-discharge. Solid-state polymer electrolyte membranes are a promising alternative to liquid electrolytes because they offer good processability and are electrochemically/thermally more stable. A key challenge is to achieve a highly ionic conductive membranes that maintain both, high-modulus and chemical/thermal stability. In the present work, the structure and conductivity of hybrid polymer electrolyte membranes composed of polystyrene-*block*-polyethylene oxide (PS-*b*-PEO) diblock copolymer (DBC), lithium salt and ionic liquid (IL) were investigated. This hybrid system has a rigid PS block and a Li-ion conducting PEO block. The morphology and crystallinity of this hybrid system as function of IL content and temperature were investigated using wide-angle and small-angle X-ray scattering (WAXS/SAXS) methods. With increasing the IL content, the PEO crystals are highly suppressed in the DBC/Li-ion/IL hybrid materials. Amorphorization of this system is desirable since the Li-ion migration is highly suppressed for PEO crystalline containing materials. A morphological transition from lamellar to hexagonally packed cylinder (HPC) morphology upon increasing the IL content was observed. The ionic conductivity of these 3-components system was investigated using impedance spectroscopy. The conductivity measurements showed a pronounced increase with increasing content of ionic liquid (figure 1). This conductivity improvement is discussed based on both the morphology and crystallinity behavior of the investigated samples.

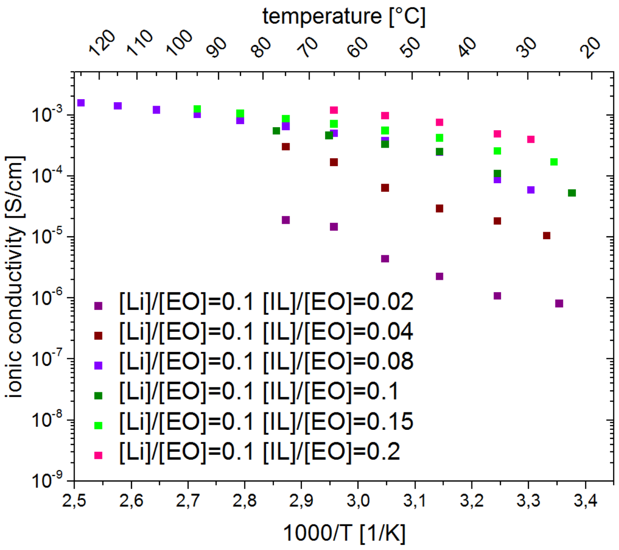

Figure 1: Arrhenius plot of DBC/Li-ion/IL hybrid materials

References:

[1] Jeffrey W. Fergus, *J. Power Sources* 195, 4554 (2010)
[2] E. Metwalli, M. Rasool, S. Brunner, P. Müller-Buschbaum, *ChemPhysChem* 16, 2881(2015).

NoFaRe: A Non-Intrusive Facility Resource Monitoring System

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Traditional indicators like monthly or annual energy consumption fail to support consumers in making intelligent decisions. To participate effectively, the consumers need to be motivated by supplying them real-time consumption information, preferably at the appliance level. Lately, the non-intrusive load monitoring (NILM) concept has gained wide popularity due to its single point sensing, user-friendly deployment, and load prediction capabilities. NILM was introduced by Hart and Schweppe in the late 1980's and their approach is based on continuously observing changes in real and reactive power consumption measured at a single point in a circuit and detecting appliance on/off switching based on unique load signatures. This was sufficient to identify the state of small residential loads with a limited number of states at accuracies up to 85%. Hart's seminal work has spawned several follow-up studies investigating the feasibility of NILM in different settings using various methods, including work on more complex loads found in commercial and industrial buildings.

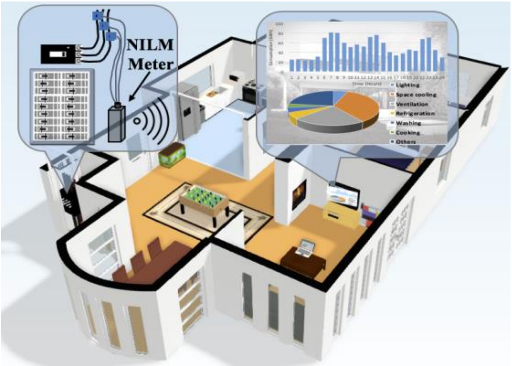

Fig. 1: Non-Intrusive Load Monitoring (NILM)

Buildings can be viewed as complex cyber-physical systems consisting of many controllable elements, e.g., doors, blinds, elevators, air conditioning units, lighting, fire protection, and various other appliances. Building management systems (BMS) are software systems for monitoring and controlling the state of building elements and rely on corresponding hardware, in particular sensors and actuators connected to a central server via a communication network. The visible part of a BMS typically includes a graphical user interface that allows building managers to remotely monitor relevant building functions and adjust controls whenever necessary. Presently, the primary challenge facing the efficient integration and interoperability of any BMS is the lack of standardization. This results in data integration and scalability issues between multi-vendor devices, making BMS vulnerable to cyber-security and privacy issues. A solution could be the realization of open control architecture, capable of running seamlessly over multi-vendor platforms and interoperable with many different applications within the BMS. The resulting system will not only be cost-efficient but also ease the process of data analytics.

In summary, both NILM and BMS research areas are attracting increasing attention. NILM could allow for low-cost device-level monitoring and turn out to be a key enabler of next generation BMS. NILM research has so far focused on accurate disaggregation, but not deployment cost, usability, or concrete applications to building management. It is thus particularly interesting to explore innovative BMS applications that can be enabled with NILM and how actual NILM processes and system architectures could look like.

The NoFaRe project will address these research gaps by developing a new NILM system including a self-designed smart meter box composed of a single-board computer equipped with a LAN/WiFi interface, a memory card, and one or multiple 16-bit A/D converters for conducting circuit measurements at high frequencies of up to 50 kHz. Our system will allow for device detection, type classification, state inference, and power disaggregation in an industrial, commercial, or private building environment. It will include a web-based management frontend that will allow for carrying out all necessary configuration, training and appliance registration tasks. Furthermore, we plan to design innovative BMS applications that leverage the NILM capabilities provided by the NoFaRe system.

e-MOBILie – Smart home energy management in residential buildings

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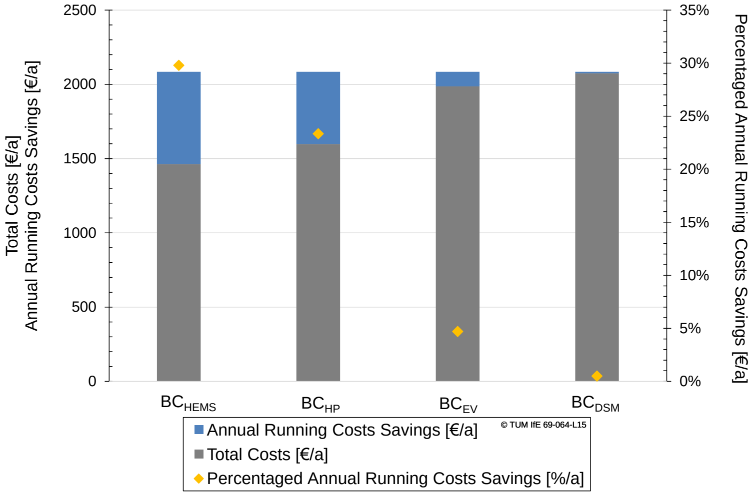
The German energy supply will face huge structural changes within the next decades. Decentralized power units on a renewable basis will steadily replace centralized energy production in power plants. However, renewable energy supply deals with uncertainties due to its intermittent character. In order to ensure equality between electrical supply and consumption at all time further potential helping this equation to balance is needed. This capacity is especially to be found on the consumer side of the energy system, as the concept of energy production being a result of consumption has to be adapted so that demand follows production. Applying this principle, called Demand Side Management (DSM), on a smaller scale, e.g. on private households, offers a huge potential with its multitude of appliances that can be time shifted. Furthermore, decentralized on-site energy production, i.e. by photovoltaic systems, does not compulsorily match demand throughout a day. Usually the external grid balances supply and load exclusively.

Home energy management systems (HEMS) are capable of reducing this discrepancy by shifting loads into times of energy surplus. Therefore, they simultaneously improve the integration of renewable energy into the grid of residential buildings and allows benefiting from variable electricity prices. The HEMS minimizes the overall energy costs whilst orientating its functionality to electricity price and weather forecast, e.g. prognosis of photovoltaic energy generation. Thus, all electrical loads, i.e. washing machine or electric vehicle (EV), and any electrical storage are arranged in a cost optimal schedule. In addition, in residential buildings where the electrical and thermal sector are combined via electric heat generators not only electrical load but likewise thermal production shifting is facilitated. As thermal storages are available in these building configurations this coupling allows variations of the thermal load.



In conclusion, it is shown that a HEMS utilizes the existing load shifting potential in a residential building for generating significant benefits regarding yearly energy costs and increase both autarky and self-consumption in a positive manner. The largest ecological and economical benefit of shifting in-house energies and loads is provided by coupling of heat and electrical sector through heat pump and immersion heater, whereas a predictive and intelligent control strategy gathers higher potential. Additional cost savings can be extracted out of intelligent controlled charging of EV, whereby a large dependency on the users' driving profile is observed. By the way, DSM devices offer only little potential due to their small share of energy and power demand and their restrictions concerning user behaviour. All studies are carried out within the project „e-MOBILie – energy autonomous electro mobility in a smart-micro-grid".

Porous titania-based hybrid films as electrodes for lithium-ion batteries

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Porous titania hybrid films are promising candidates as electrodes for lithium-ion batteries [1]. Large surface area of nanoporous titania/Si nanoparticles (NP) and TiO_2/SiO_2 hybrid films enables both, high current density and improved cycling behavior. The block copolymer assisted sol-gel templating technique was used successfully to prepare nanoscale porous electrodes. Amphiphlic polystyrene-*block*-polyethylene oxide (PS-*b*-PEO) diblock copolymer was used as a structure directing agent to create both, foam-like and ordered cylindrical mesoporous TiO_2/Si-NP and TiO_2/SiO_2 hybrid films via this sol-gel method [2]. The morphology of the porous hybrid films was probed using SEM and small-angle X-ray scattering (SAXS). The crystallinity of the titania films was systematically measured as a function of the silicon NP content using X-ray diffraction (XRD). The TiO_2/Si-NP hybrid films are tested as electrodes for lithium-ion batteries showing a unique combination of both, the high capacity and the resistance to the lithium dendrites formation.

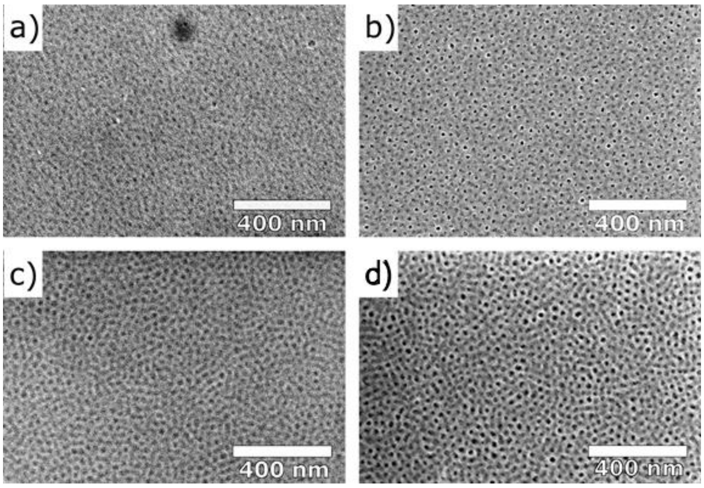

Figure 1: SEM image of nanoporous TiO2/SiO2 hybrid films with a 0.5 TiO_2/SiO_2 ratio. The PS-*b*-PEO diblock copolymer was used as a template with a composition of a,b) 15.5-*b*-35.5 kg/mol and c,d) 20.5-*b*-8 kg/mol. a,c) before, b,d) after calcination at 400°C

References:

[1] S. Goriparti et al., *J. Power Sources* 257, 421 (2014).
[2] M. A. Niedermeier et al., *Nanotechnology* 23, 145602 (2012).

First-Principles Embedded Cluster Calculations of Surface Defects at TiO_2 (110)

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Bulk and surface defects critically determine many of the properties and functions that make TiO_2 such an interesting and widely studied material. Given this importance, it is both surprising and discomforting to see how little is actually known especially about the surface defects of TiO_2. For surface oxygen vacancies not even their thermodynamically favored charge state is unambiguously clear. We contribute to this context with first-principles embedded cluster calculations [1] of the rutile TiO_2 (110) surface. Our approach allows for a numerically particularly efficient application of hybrid density-functional theory inside the quantum mechanic (QM) cluster region. In the extended molecular mechanic (MM) embedding region specifically optimized interatomic potentials provide a quantitative account of the strong TiO_2 polarization response. We present the advantages of this QM/MM approach against more common periodic supercell calculations especially for charged O vacancies. Over a wide range of electrochemical potentials and oxygen partial pressures our calculations show [2] the +2 state to be thermodynamically favored, which can be rationalized by the huge dielectric constant of TiO_2.

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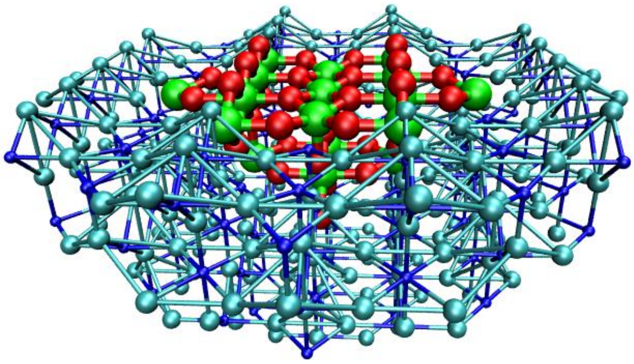

Energy Demand Reduction of Public Properties

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The HoEff-CIM project ("Energie**Eff**iziente **Ho**chschule – **C**ampus **I**nformation **M**odeling", engl. "Energy-Efficient University – Campus Information Modeling") shows how to support universities in creating a climate-neutral building stock by demand reductions and efficiency improvements based on the example of the campus of the Ludwig-Maximilians-Universität München (LMU). The aim of this project is to realize a good opportunity to determine energy saving potentials of public properties by identifying their current demand and giving sustainable retrofit possibilities.

The project partners define ways to reduce energy demands and improve the efficiency of universities and public properties by using an interactive and holistic information-model. Therefore, a web-based tool will be developed, which simplifies the identification of current demand and gives first valuable advices for a more efficient building stock ("QuickCheck-Tool").

Especially universities have heterogeneous usage profiles, like offices, laboratories, or lecture rooms with different energy demand. In addition, the building age spans from before 1918 until recently built buildings. Historic structures of the building envelopes of the LMU are categorised in ten age-of-building classes. Figure 1 shows the distribution of buildings over the different age-of-building classes and the entire retrofit according to current energy standards. In addition, it shows the final energy demand for each age-of-building class.

To guarantee comparable results a representative building of the LMU was developed in order to compare the different restoration actions and their saving potentials of each component. Figure 2 shows the potentials of each component for a nearly-zero energy standard. The green line shows the total retrofit of the representative building (41 kWh/(m²a)).

Afterwards each energy consumption or demand is compared with the saving potential regarding to current (German "EnEV 2014") and prospective (nearly-zero) energy standard. The results of the building physics will later be associated with the building services and the buildings use.

As an overall result, sustainable (energetic, economic and environmental) retrofits can be defined for each building-age-class or usage profile.

The project is funded by the German Federal Ministry for Economic Affairs and Energy and will be completed in summer 2017. For more information please refer to www.hoeff.info.

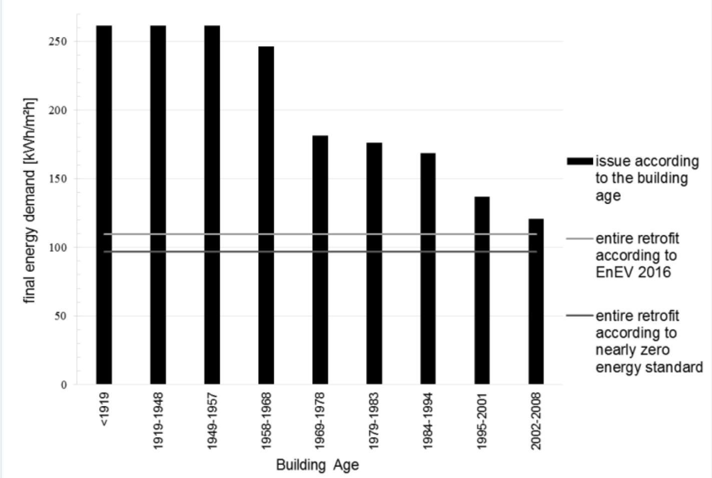

Figure 1: Issues according to the building age and final energy demand

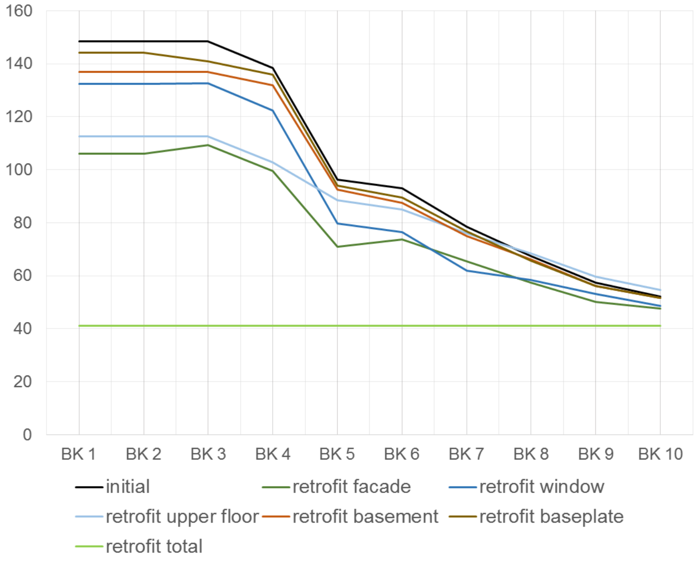

Figure 2: Energy saving potential of each age-of-building class by component

Influence of the drying process on the mechanical and electrical properties of electrodes for Li-ion batteries

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The drying process of lithium-ion battery (LiB) electrodes is carried out in a variety of ways, for example using convection ovens, air-flow-generating drying nozzles[1] or infrared radiation. In industry, electrodes are often dried in a continuous way using infrared radiation. However, the temperature during the infrared drying process strongly affects the mechanical and electrical properties of the electrodes, such as adhesion, which is a key parameter for the quality of LiB-electrodes.

The goal of our current research is to investigate the influence of the drying process with infrared radiation at different temperatures on the mechanical and electrical properties of electrodes for lithium-ion batteries. Of particular focus will be the influence of the solid content of the coating inks on the distribution of the polyvinylidenefluorid binder (PVDF) across the dried electrodes.

The electrodes (dried with an inhouse IR-drying system) consist of LFP as active material, PVDF as binder, and carbon black as conductive additive, at a composition 90/5/5 (LFP/PVDF/carbon). The solid components are mixed with 1-methyl-2-pyrrolidinone (NMP) as solvent, at amounts resulting in solid contents ($\equiv m_{solids}/(m_{solids} + m_{NMP})$) of 40 %, 50 %, 60 %. Inks are coated on an 18 µm aluminium foil at a loading of ~ 10.5 mg LFP/cm^2_{geo}.

The coatings are dried with infrared radiation for 10 minutes at different average temperatures of 60 °C, 80 °C, 100 °C and 120 °C, followed by drying at 50 °C in an air-circulation oven. During the IR-drying process, the power of the infrared source and the distance to the sample is held constant.

We will show results on the coating adhesion and contact resistances of the electrodes, and correlate their dependence on the drying process. Furthermore, the surface is analyzed via IR-spectroscopy to indicate the PVDF (binder) distribution in the electrode. The aim of the investigations is a better understanding of the electrode's micro structure and to find the optimum parameters of the drying process.

Literature:

[1] B. Westphal, H. Bockholt, T. Günther, W. Haselrieder and A. Kwade, *ECS Trans.*, **64**, 57–68 (2015).

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Optimized control and condition monitoring of electric submersible pumps (ESP) in geothermal power plants

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Electricity production using geothermal power systems might be a promising supplement to sustainable energy production in the future as base load power can be provided and the thermal energy capacity of the earth can be considered effectively unlimited [1, p. 2].

The Southern German Molasse Basin shows great potential for geothermal power systems as it is one of the largest reservoirs for geothermal energy within Central Europe [2]. The water temperature in the Malm aquifer of the Molasse Basin reaches profitable values (>120°C) at drilling depths of 3000-3500 m [1, p. 155 ff.]. In these so called low enthalpy regions, typically hydrothermal doublet systems are used, which consist of two spatially separated wells, the production well and the injection well. The former extracts thermal water from the aquifer, while the latter reinjects the cooled water from the power plant. For electricity production in the lower temperature regions, binary systems such as Organic Ranking Cycle plants (OCR) or Kalina plants are employed, which use heat exchangers at the surface to transfer heat from the primary fluid (thermal water) to a secondary (working) fluid with favourable steam production properties: Contrary to water, the working fluid evaporates nonisothermally which effectively results in a higher steam temperature and hence in an increased Carnot efficiency $\eta_C = 1 - T_{low}/T_{high}$ [1] of the process, with T_{high} [K] and T_{low} [K] being the temperature of the steam entering the heat engine and the waste heat, respectively [3, p. 245 ff.].

Despite its initially mentioned advantages, a geothermal system poses serious challenges concerning mechanical, thermal and chemical stresses of its components, in particular of the electric submersible pump (ESP) responsible for the transportation of geothermal fluid from the aquifer to the surface [1, pp. 46,47]. Due to the fact that the submerged pump is located at great depth and hence not easy to access, high reliability is essential for economical operation of the system. As a consequence, one of the major challenges is to increase the lifetime of the pumps.

Various fields of research may contribute to achieving this goal, e.g. mechanical engineering or material sciences may produce reinforcements of single components or the mechanical setup. But also from the control theoretic perspective improvements can be expected, which will be the main focus of this research project. Using a model based approach, a detailed mathematical model of the ESP, the power electronics and the sensor system will be derived in the first step. Based on this model, a control system will be developed, considering objectives like fault protection and efficiency enhancement. Moreover, a condition monitoring system will be developed, allowing for early warnings of imminent system faults and improved maintenance scheduling. Desired outcome of this project is furthermore a modular simulation environment of the pump system, for practical application in research and industry.

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Solution-processed insoluble polythiophene for organic solar cells

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Since the discovery of conjugating polymers in the 1970s their synthesis and the development and optimization of applications has been in the focus of research. Since their conductivity and optoelectronic properties strongly depend on the molecular morphology and crystallinity, controlling the thin film morphology is one of the main challenges when it comes to developing fabrication processes that work on small labs as well as in large industrial scales. As many conjugated polymers are insoluble in most common solvents and do not allow processing directly from solution, they are often equipped with solubilizing side chains. While these enhance the polymer solubility, they can also lead to unwanted twists in the polymer backbone. Thereby the conjugation length and degree of crystallization can be decreased resulting in altering conductivity and optoelectronic properties of the polymer.[1]

In situ polymerization offers the possibility to process polymers from solution without the need for solubilizing side chains. For this purpose, the corresponding monomers are deposited onto the substrate and chemically linked afterwards. This way the amount of electrically insulating molecular parts in the film are reduced to a minimum. Moreover, the insolubility of the resulting semiconducting films leads to an increased stability against external impacts and offers new possibilities of structuring the polymer film.

In this work, polythiophene (PT) films for active layers of organic solar cells are synthesized *in situ*. Bithiophene, the soluble monomer, is deposited to the corresponding substrates and linked by an oxidative polymerization reaction.[2] The PT acts as main light absorber and electron donor within the solar cell. Furthermore, a fullerene derivative (PCBM) is implemented into the active layer structure to serve as acceptor material. The simplest architecture, in which the active layer can be build, is a bilayer of the two materials as shown in figure 1. Here, the layers of polymer and fullerene are stacked above each other with negligible intermixing of the two materials.

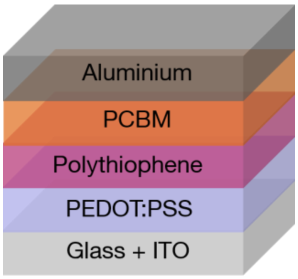

Figure 1: Bilayer stack of investigated solar cells.

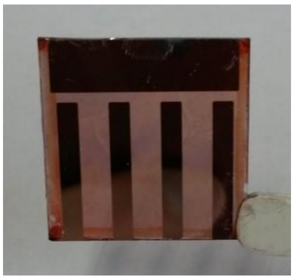

Figure 2: Lab scale PT/PCBM organic solar.

For efficient light-harvesting as well as charge carrier generation and transport processes, the interface between the two components, polymer and fullerene, needs to be highly enlarged in comparison to the bilayer. By structuring the polythiophene with a removable template during the polymerization process, it is possible to obtain a porous morphology with structures on the nanometer scale. A systematic variation of the template size allows a detailed investigation of the influence of the interfacial area on the device performance. The insolubility of the synthesized polythiophene assures the stability of the structures even during the backfilling from PCBM solution.

The different thin films are investigated regarding their interaction with light by measurements of absorbance and photoluminescence, their charge carrier mobility and their performance in solar cell devices, to obtain an insight on the influence of the interfacial area.

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Activation of Silicon Electrodes for the (Photo-) Electrochemical CO_2 Reduction

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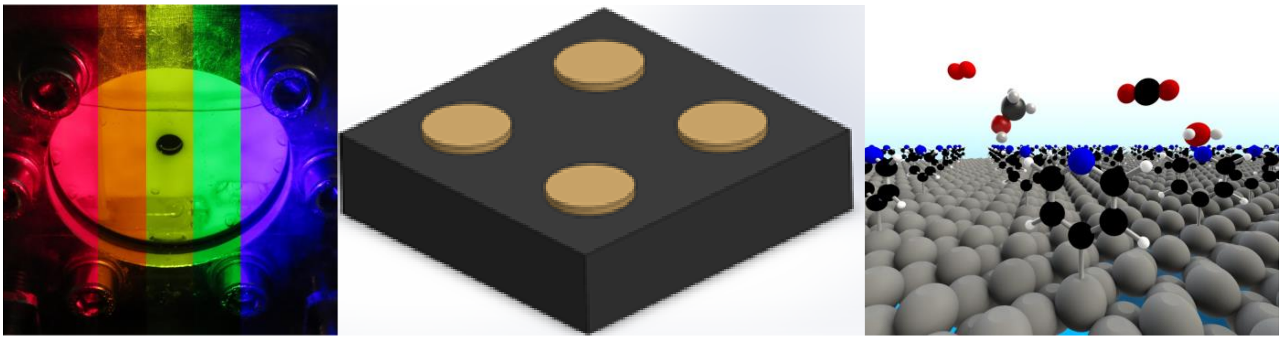
CO_2 conversion to fuels or basic chemicals in a photo-electrochemical cell is an attractive route to store solar energy in chemical bonds while also using the main combustion product carbon dioxide as a feedstock. Attempts to create such an "artificial leaf" have to deal with the large activation barrier of CO_2 reduction which tends to lead to low yields and efficiencies.

Using silicon (Si) photoelectrodes which bandgap is ideally suited for efficiently absorbing solar light, we set out to modify its surface with catalytic components tailored for the (photo-) reduction of CO_2. We focus on two systems:



I. It is well-known that bulk metal electrodes, e.g. gold or copper, reduce CO_2 at high overpotentials [1]. Typical products are CO, ethylene and methane. Our aim is to integrate such metal catalysts ontop our photoelectrochemical Si electrode as reaction centers for the CO_2 reduction. We realize such a system by structuring a silicon substrate with chessboard arrays of gold nanodisks. They can be electrochemically plated by copper which is the only material known to reduce CO_2 to methane and ethylene.

II. It has been known for some time that dissolved pyridine has a catalytic effect on the reduction of CO_2 to methanol on platinum and p-GaP electrodes [2,3]. However, so far the overall reaction mechanism is not understood. Using electrochemical methods such as cyclic voltammetry and rotating disk electrolysis, our group investigated the electrochemical behavior of dissolved pyridine on Pt. Our experiments revealed clear indications for the contribution of adsorbed pyridine species in the CO_2 reduction mechanism. Inspired by the catalytic effects of dissolved (and/or adsorbed) pyridine on reduction of CO_2, we demonstrate that a functionalized p-Si electrode constitutes a promising interface for the photoelectrochemical CO_2 reduction. The interface consists of pyridine molecules which are immobilized on the Si surface via an electrografting process [4].

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Fe/activated-graphene based ORR catalysts: synergistic effect of N/S/P

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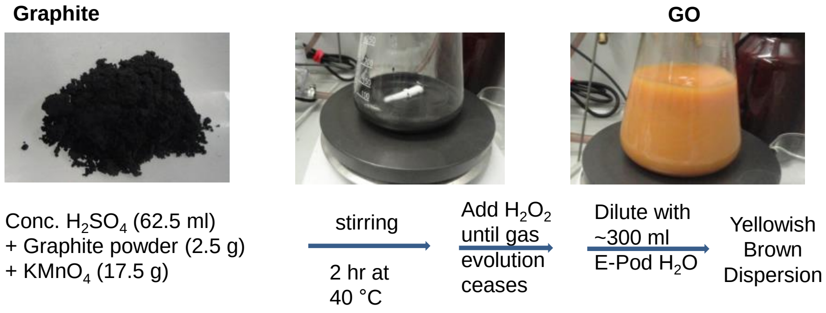
Non-noble metal catalysts for the Oxygen Reduction Reaction (ORR) have been investigated as a replacement for platinum-based catalysts over the last five decades. The motivation to replace platinum-based catalysts is their high cost and limited availability, which is a major hurdle towards the commercialization of Proton Exchange Membrane Fuel Cell (PEMFC) systems. Until today, Fe-N-C based catalysts are the most active state-of-the-art non-noble metal catalysts [1]. At present, research is heading towards increasing the activity and stability of Fe-N-C catalysts. In parallel to catalyst activity and stability improvement, research on alternative catalyst supports is also getting increased attention, e.g., graphene based supports due to their high electrochemical stability and the possibility to integrate various heteroatoms like N, S, P, etc., in the graphene structure [2], which alter its chemical properties [3]. On the one hand, it is well known that Fe coordinated with N and C significantly affect the ORR activity [1], while on the other hand it is also interesting to examine whether addition of S- and/or P-dopants could lead to any synergistic effect between these heteroatoms and Fe. In our study we have investigated Fe-based catalysts with N-, S-, and P-heteroatoms and activated graphene as a support.



Conc. H_2SO_4 (62.5 ml)
+ Graphite powder (2.5 g)
+ $KMnO_4$ (17.5 g)

stirring → 2 hr at 40 °C

Add H_2O_2 until gas evolution ceases

Dilute with ~300 ml → E-Pod H_2O

Yellowish Brown Dispersion

Figure 1: Synthesis of graphene oxide (GO) from graphite [4]

Graphene oxide (GO) was first synthesized by a modified Hummers method [4], and then it was heat-treated with KOH to yield activated graphene support [5]. Further, a series of samples with various permutations of Fe and heteroatoms were synthesized. This was followed by structural characterization with BET, TEM, Raman, elemental analyses, etc. Electrochemical characterization was done in a thermostated standard three-electrode glass cell. All the measurements were done using the thin-film rotating disk electrode (RDE) technique at 20 °C in 0.1 M $HClO_4$ electrolyte [6]. Results from the structural and electrochemical characterization assist in answering the aforementioned question about synergism, pointing towards future catalyst development strategies.

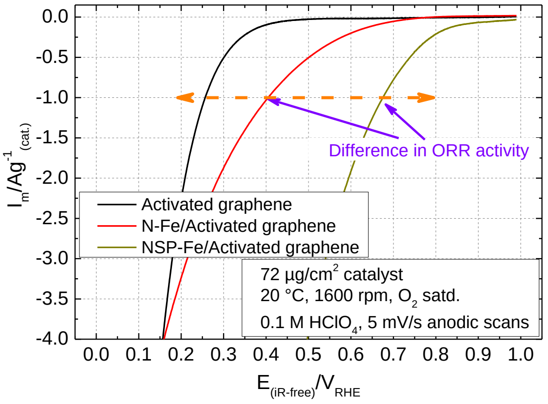


Figure 2: ORR mass activities of heteroatom integrated samples in 0.1 M $HClO_4$ at 20 °C

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MIS-CELIV: A novel technique for measuring charge carrier mobilities

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In order to keep up with the growing world energy consumption and the need for clean energy sources, it is important to develop new techniques for energy harvesting. One of the recently emerging and challenging fields of research are organic photovoltaics, which consist of semi-conducting polymers. This material class offers new possibilities and advantages over the traditional silicon solar cells. Due to their high absorption ability, only thin films of hundreds of nanometres are necessary, making them light-weight and flexible. Another advantage is the fact that semi-conducting polymers are solution-processable which allows the sample fabrication to be shifted from lab scale to big manufacturing processes like roll-to-roll processing.

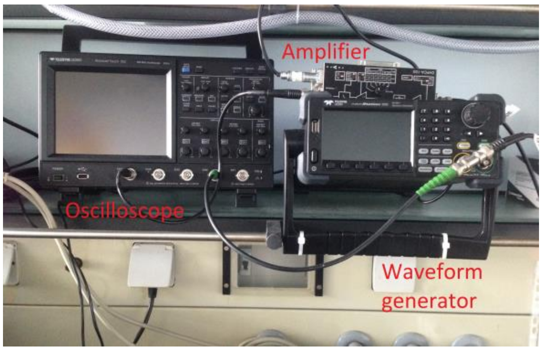

Figure 1: The setup for the MIS-Celiv including the oscilloscope, the wave form generator and the amplifier.

However, the efficiency of organic solar cells is relatively low. This is partly based on the fact, that many characteristics and properties of this new material class are still not fully understood. However, it is by now well established that the performance of organic solar cells is strongly linked to morphology. The morphology and therefore the properties of organic solar cells can be influenced by manipulating certain parameters in the fabrication process of these thin films.

One of the key performance parameters of semi-conducting polymers is the charge carrier mobility. Measuring the mobility of charge carriers is an important step in assessing the efficiency of organic solar cells. The charge carrier mobility can be determined using various different methods. One of these methods is the MIS-CELIV. This technique represents a **M**etal-**I**nsulator-**S**emiconductor architecture, where **C**harges are **E**xtracted by **L**inearly **I**ncreasing **V**oltage. It is a suitable method for organic thin films, as it allows selective measurement of both electron and hole mobilities [1]. Measurements can be conducted as well on the semiconducting materials itself or on any blend mixture, making it a sophisticated method, to obtain information on active layers that represent the operational solar cell devices.

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In-plane and cross-plane Seebeck coefficients in hybrid thermoelectric films

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As energy demand around the world increases and the amount of non-renewable fossil fuels decreases, the need for sustainable renewable energy sources is evident. In addition to the growing demand for energy, there is also a push for reducing the amount of emitted pollution, in the form of greenhouse gasses, by using clean energy sources. Thermoelectric materials (TE) convert heat directly into electricity. This clean energy technology has advantages over other renewable technologies in that it requires no sunlight and has no moving parts. With the majority of the unused energy in the world being wasted in the form of heat and the recent mandates to reduce greenhouse gas emissions, thermoelectric devices could play an important role in our energy future by recovering this wasted heat and increasing the efficiency of energy production.

The Seebeck effect describes the generation of a voltage across the material as function of the applied temperature gradient. So far, semiconducting ceramics have been mostly used as highly efficient TEs. However, the materials mostly used comprise rare/toxic/expensive materials such as lead, tellurium, bismuth, etc. Thus, conducting polymer materials are attractive TEs due to their intrinsically low thermal conductivity and relatively high and tunable electrical conductivity. Still, similar challenges regarding optimization as in their inorganic counterparts remain, due to the complex interplay of the thermoelectric parameters, namely Seebeck coefficient, thermal and electrical conductivity.

In this investigation, we study the influence of different nanostructuring procedures on in-plane (temperature gradients along the film surface) and cross-plane[1] (perpendicular to film surface) thermoelectric properties of PEDOT:PSS thin films. PEDOT:PSS is a commercially available and water-soluble conducting polymer with tunable electrical conductivity. Sketches of the different architectures can be seen in Figure 1.

In cross-plane investigations, we have achieved high Seebeck coefficients with values of up to 128 µV/K in a relatively low temperature range using the commercially available conducting polymer blend PEDOT:PSS in a hybrid metal/polymer/metal thin film device. In addition, we managed the fabrication of PEDOT:PSS thin films on flexible PET substrates and measured in-plane Seebeck coefficients of up to 11 µV/K. Continuing research in this area, we attempt to enhance the Seebeck coefficient even further by optimizing the thickness and post treatment of the PEDOT:PSS thin film and also using different materials as inorganic components. In addition, grazing incidence scattering experiments should reveal structural implications of the hybrid architecture on the polymer morphology. We are going to link this to the thermoelectric properties of the hybrid devices.

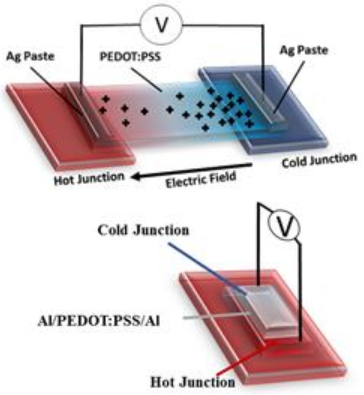

Figure 1: Schematic of in-plane(top) and cross-plane (bottom) Seebeck measurement setup

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Iridium oxide catalysts for electrolysis applications

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Energy storage is undoubtedly still a great challenge, especially for excess energy obtained from renewable sources such as solar and wind energy. Hydrogen is by far the most promising option as sustainable energy carrier. For a clean, fossil- and CO_2- free hydrogen production, proton exchange membrane (PEM) water electrolysis was recognized as a key technology which fulfills the ever increasing demand for green energy.

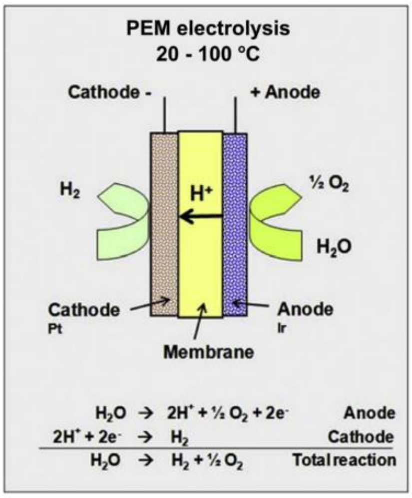

Figure 1: PEM water electrolysis.[1]

In a typical electrolysis process, electricity and water are converted into hydrogen and oxygen. The acidic environment during water splitting in the electrolyzer makes the use of platinum-group metals (PGM) as electrocatalysts unavoidable, which adds significantly to the overall cost and therefore represents the major drawback of this technology.

In order to make PEM water electrolysis more cost affordable, many efforts were devoted at reducing the catalyst loading. For hydrogen evolution reaction (HER), a great improvement was achieved by supporting Platinum on a carbonaceous support. For oxygen evolution reaction (OER), Iridium oxide is by far the most active and most studied catalyst, but reaching low loadings is more challenging. Different approaches to reduce the Iridium loading include the dispersion of Iridium oxide nanoparticles on a support and the application of nanostructured core-shell materials.

We have investigated the OER activity on different catalysts made by a chemical reduction method, specifically, using the polyol method. This method provides a facile synthesis of metal-containing compounds in ethylene glycol, which acts as both solvent and reducing agent.

Iridium nanoparticles of controlled size and shape were synthesized and deposited on either Titanium oxide or Antimony-doped Tin oxide (ATO) to form the targeted oxide-supported Iridium catalyst. Another catalyst was prepared by mild oxidation of the already supported Iridium catalyst to result into oxide-supported $\text{Iridium}_{\text{core}}$ - $\text{Iridium oxide}_{\text{shell}}$ catalyst. Hereby one focus of this study was the effect of Iridium core and Iridium oxide shell thickness on the activity. The third investigated catalyst was prepared by full oxidation of the already supported Iridium catalyst to result into Iridium oxide nanoparticles supported on oxide substrates. All catalysts were characterized by XRD, BET and TEM.

The OER activity of the three investigated catalysts was investigated by using rotating disc electrode technique and the results were compared to commercial supported Iridium oxide catalysts. The difference in the activities of the three investigated types of catalysts will be explained and correlated to the oxidation states of both, Iridium and the metal of the oxide support.

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Power exhaust in a nuclear fusion reactor and the possibility to use W-Cu composites as heat sink materials for highly loaded plasma facing components

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The design and realisation of a power producing nuclear fusion device comes with great challenges. One of the major challenges that is distinctly depicted within the roadmap to the realisation of fusion electricity published by EFDA [1] is the challenge of power exhaust. In order to maintain high temperature plasmas in a nuclear fusion reactor, large particle and heat fluxes have to be exhausted in a rather narrow region of the reaction chamber. The corresponding plasma facing component (PFC) that must be capable of withstanding these loads is called the divertor. The performance of such a highly loaded PFC is most closely linked to the properties of the materials that are used for its design. Against this background, the development of advanced materials with adequate properties is mandatory in order to extend the performance of divertor targets where during operation heat loads of 10 MW/m2 – 20 MW/m2 have to be removed continuously and reliably.

One promising class of materials intended for heat sink applications in highly loaded PFCs are W-Cu composite materials [2]. These materials exhibit a favourable combination of material properties, i.e. a high thermal conductivity due to a coherent Cu matrix, enhanced mechanical properties at elevated temperatures due to W reinforcements, as well as the possibility that macroscopic material properties can be tailored by customising the composite microstructure.

On the one hand, the contribution will point out what the technological implications of the issue-area of power exhaust in a future nuclear fusion reactor are. On the other hand, the contribution will report on current development efforts regarding melt infiltrated W-Cu composite materials that are considered as advanced heat sink materials for divertor targets.

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Morphology and performance of Organic Solar Cells studied with *in-operando* scattering techniques

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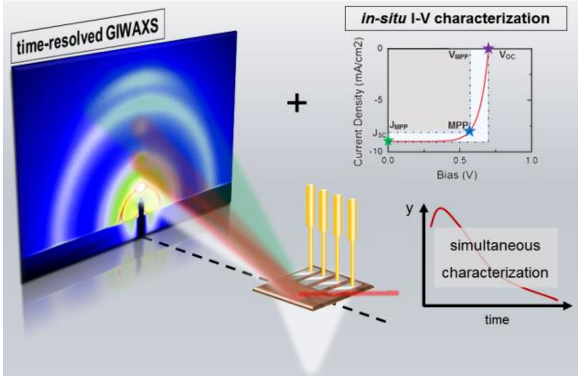

Figure 1: Schematic depiction of the setup of an *in-operando* GIWAXS experiment featuring simultaneous electronical and crystalline characterization

Organic photovoltaics (OPV) features a promising technology in the new energy generation strategies resulting from the "*Energiewende*". After just few years around, organic solar cells (OSCs) are starting to achieve efficiencies and lifetimes that make them competitive compared to other classical solar technologies and render them a potential solid share of the future energy generation schema. They present as well other features like light-weight, semi-transparency and low fabrication costs, making the also suitable for a full new range of applications where green energy generation was still not broadly present.

Further effort on raising efficiencies and lifetimes of these devices, as well as lowering their costs, is one of the mainstream lines in organic photovoltaics research. In this regard, it is already long stablished that many of the features that devices present in their functioning are intimately related to the specifications of the morphology of the films composing them. Careful study of the links between morphology and performance over the past years has already yielded deeper insight into the physics governing excitonic solar cells.

Recently, OPV research has started also to seek for a deeper understanding of the ageing processes that shorten device lifetimes and their link to changing film morphology. In this regard, one of the most innovative approaches consists of the *in-operando* observation of solar devices under working conditions in time-resolved grazing incidence X-ray scattering experiments. This configuration allows for simultaneous tracking of morphological and electronic properties as a function of time, making the appearing co-dependences among studied parameters more remarkable.

The presented work focuses on the first *in-operando* observations that showed strong correlations between the crystalline state of P3HT:PCBM OSCs' active layers and the open-circuit (V_{OC}) voltage delivered by the devices. Until now, this link was only addressed in a multi-step fashion with works featuring separate interdependences between properties like crystallinity, recombination, energy disorder, open-circuit voltage, or exciton/charge carrier transport. Now, the *in-operando* observations help spotting correlations between the different implied parameters, providing an inside look on the changes worsening device performance as well as improving fundamental physics, material and device understanding.

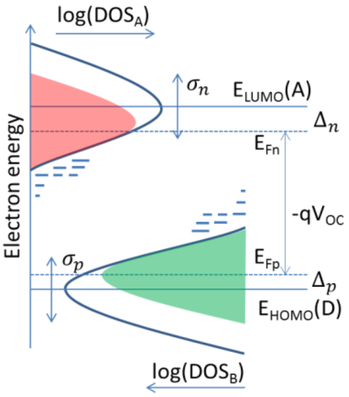

Figure 2: Sketch of the distribution of the relevant energy features involved in the creation of a photovoltage in a working OSC

Energy State Model for Bottling Plants

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Modern bottling companies focus on green value. Currently there are disparities regarding the specification and analysis of energetic behavior of new and existing machines. Machine efficiency and energy consumption are often intermixed (e.g. kWh/ 1000 fillings). In this work an energy state model is presented to describe the energetic behavior of machines generically in order to achieve more comparability. The central idea of the model is, that the energetic behavior of a machine can be described with a finite number of steady energy consumption levels depending on its operational state. Transition from one consumption level to another can be mapped simplified with an average consumption value. Data analysis of ten machines of a bottling line showed, that the energetic behaviour of all machines can be described with four main consumption level: Production, High Level Standby, Low Level Standby and Inactive. Production is a constant consumption levels a machine reaches during its production period. High Level Standby and Low Level Standby can be reached during an unplanned production stop (e.g. equipment failure) and are distinguished by production availability after the stop (minimal technical possible time or with delay). Inactive is the minimal consumption level reached during the nonproductive time. The model can be expanded by machine specific energy levels if necessary (e.g. for cleaning). The presented model can be used for specification as well as for analysis and was developed in cooperation with the German VDMA and leading German companies for bottling plants. The results will be publish in a VDMA-recommendation.

La_2NiBi – A new ternary ordered version of the Bi_3Ni structure type

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A new ternary compound of the Bi_3Ni structure type was found. La_2NiBi crystallizes isostructural to the literature known La_2NiSb in the space group type *Pnma*. For the synthesis of La_2NiBi the elements were pressed and heated in evacuated, sealed silica tubes up to 1070°K. The structure was determined via powder and single crystal X-ray diffraction.

La_2NiBi forms infinite nickel zig-zag chains along the *b* axis, which are surrounded trigonal-prismatically by lanthanum atoms. Two of the tree rectangular faces are plane-connected to further prisms and the remaining one is capped by a bismuth atom.

Furthermore, the new compound was characterized via Seebeck, conductivity and magnetic measurements.

Structuring of thin films for application in organic photovoltaics

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Thin polymer films converting light into electrical energy have recently exceeded the 10% power conversion efficiency limit [1], thus raising the interest in research for organic photovoltaics. Apart from the potentially low-cost and large-scale production, the use of flexible substrates extends the applicability of organic solar cells. Due to the low power conversion efficiencies, organic photovoltaics are still not competitive with conventional solar cells. Several methods have been described to enhance the cell performance, including the utilization of high-efficiency materials and nano-structuring of the polymer film surface.

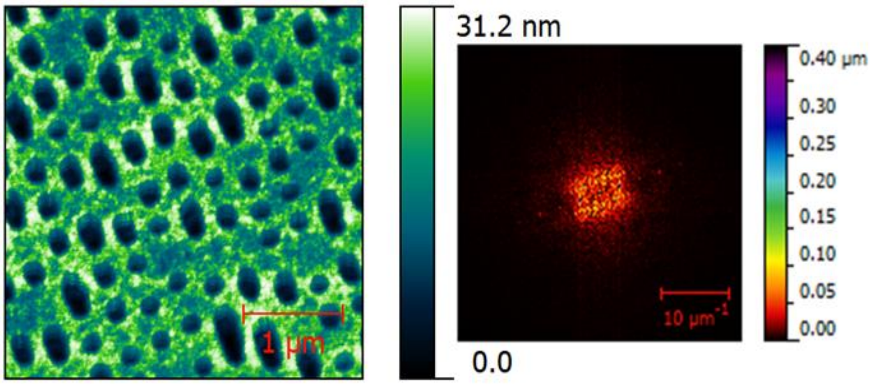

Figure 1: AFM image of imprinted active layer (left), 2 dimensional Fourier transformation of AFM image (right)

In the present study we aim to enhance light harvesting and the charge carrier separation by combining the use of low band gap materials with nano-structuring the active layer by soft embossing methods. Since the fabrication of masters with nano-scale sized structures suitable for light management is very expensive, we use patterns of compact discs and Blu-ray discs, which can be acquired at comparably low costs due to their mass production.

The optical properties of the high efficiency polymer active layer thin films are investigated using UV/Vis and photoluminescence measurements. Structural studies include optical and atomic force microscopy and X-ray diffraction methods. Prototype solar cells are manufactured and their characteristic parameters investigated.

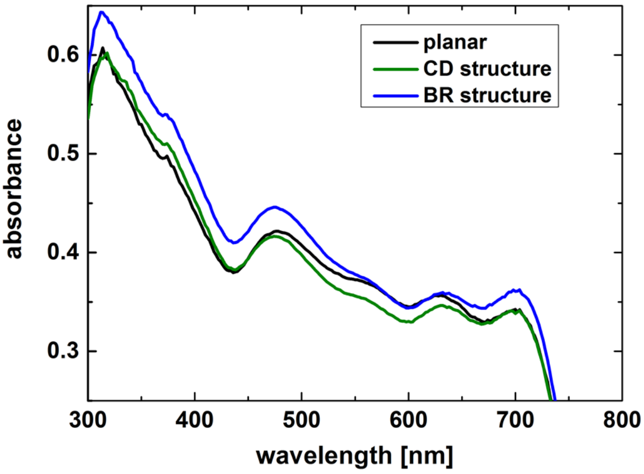

Figure 2: Absorbance measurements on planar and structured active layer films

It has been reported, that the quasi-random arrangement of pits and islands on commercial Blu-ray discs, which originally serve for high data compression, is also suitable for photon management on organic solar cells [2]. With 2D Fourier transformation of the AFM images revealing insight into the frequency space, we want to explain the differences in absorbance and reflection of differently structured active layers.

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Eco-Friendly Railway Air Conditioning

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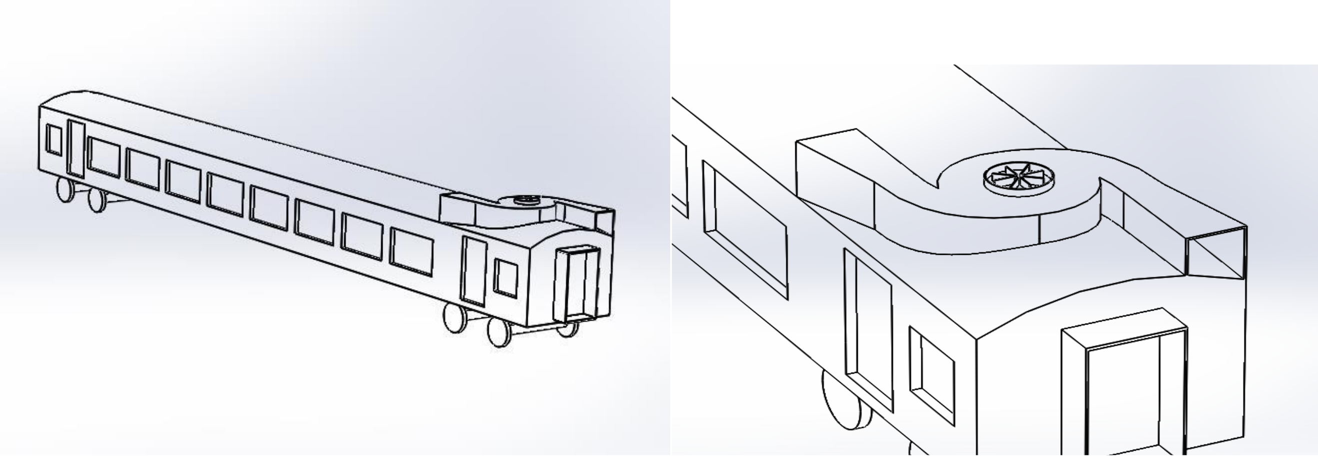
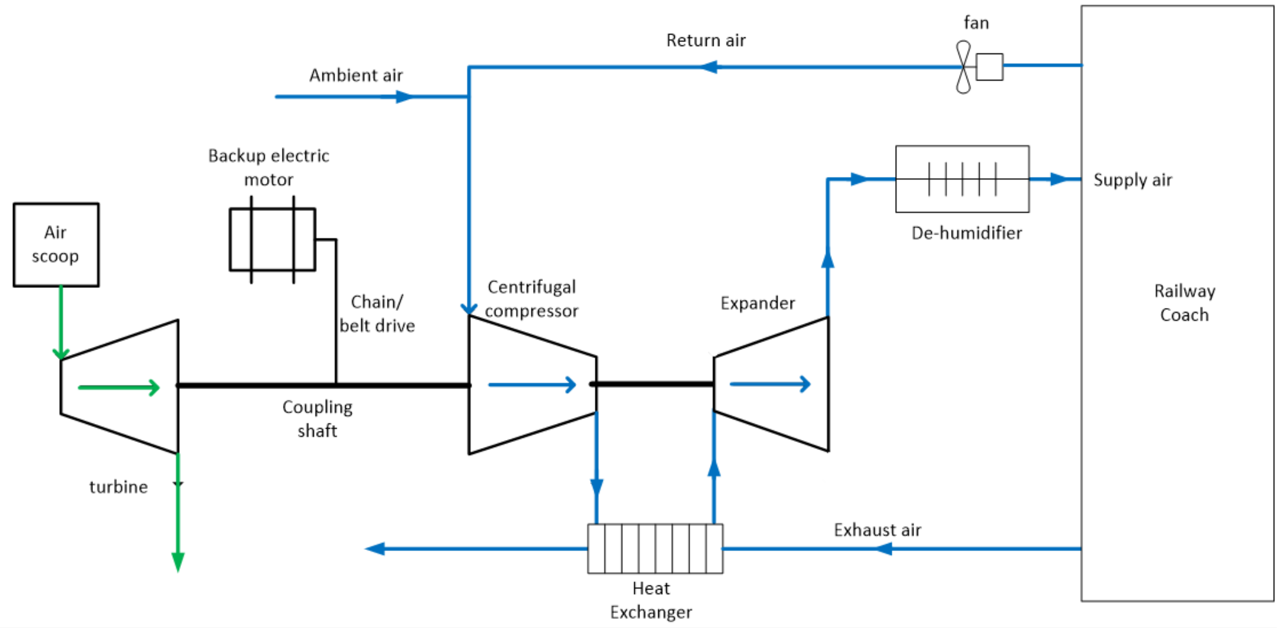
A novel eco-friendly air conditioning system has been envisioned for Indian railway coaches. The system is intended to harness the kinetic energy of wind flowing past the bogies, as the train moves. The kinetic energy is transformed into useful power by means of a radial inlet, axial exit turbine (similar to those used in automobile turbochargers). In this design, an air refrigeration cycle replaces the conventional vapour compression cycle to provide the necessary cooling in the compartment. In this paper, a preliminary analysis of the air refrigeration cycle is carried out to calculate the power requirement of the compressor. Based on the calculated power requirements, a turbine is designed. The designed turbine is found to generate sufficient power to drive the refrigerant (air, in this case) compressor.





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Design-engineering-based and material-based improvement of precast concrete facade elements

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Fig. 1: Evaluation of the test surfaces / EBB

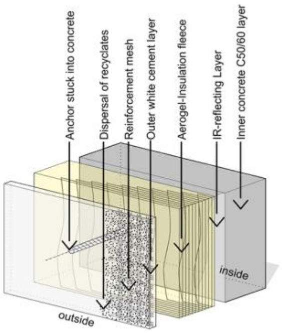

Fig. 2: Construction of the element / EBB

The interim analysis of the research project is finalized: Comparing to the production on site, precast production conditions permit the creation of more complex and higher performance building elements. Applying these optimal industrial conditions, we have the possibility to produce concrete with more organic, renewable constituents and to create building elements that are more efficient by volume.

Load-bearing behavior

-Load-bearing effect - composite shell or load-bearing inner shell: As a consequence of the analysis of reference projects, composite inner and outer shell structure is not sensible.

-Connection of outer and inner shell: Material and form: Anchor extraction tests show that a spiral form, fluted glass fiber with a chamfered end offers the best force transfer characteristics. It is structurally sufficient when the anchors are arranged perpendicular to the transfer load, an additional diagonal anchor is not necessary.

-Concrete composition: The load-bearing effect of the outer shell with variable thicknesses has been tested for the different concrete strengths for building of 5 to 6 storeys. Initial trials with UHPC showed that this material, due to its very short workability period in a fully automated work process, is not suitable for mixing in large concreting quantities. As a result, the testing reverted to the highest performance standard concrete, grade C50/60.

-Reinforcement - Material and Form: The first concrete sample elements used steel fiber reinforcement of (l/d) 09/0,15 (202,0 kg/m3). A square mesh reinforcement (round bars of d=6mm) was proposed for use with the C50/60 concrete.

-Compression test: Regardless of the thickness of the walls, the eccentricity was initially limited to 1cm top and bottom. Therefore, it is recommended to select an inner wall thickness of at least 8cm; a thickness of 9cm is optimal as it provides with greater eccentricity. Calculations revealed a required thickness of 3cm for the outer shell.

Material performance characteristics

-Insulation: Material and Form: Aerogel fleece mats offer a similar coefficient of thermal conductivity along with substantially lower vulnerability. Due to the very low volume of production, the cost of these mats remains relatively high. However, a reduction in costs can be expected with the increased demand and production.

-Avoidance of solid sections through the use of filling materials: As part of the research of the dimensioning of the inner loadbearing layer, the incorporation of additional insulation between the reinforcement anchors of the inner and outer shells was studied. This arrangement did not result in any concentration of the transmission of forces in the ribbed area provided for this purpose and therefore also no increased insulation in the infill area [1].

-IR-reflecting layer: The use of IR reflecting foil will reduce the thermal transmission and will improve the insulation of about 0,3m2K/W [2].

Surface engineering

-Concrete: Outer shell: white cement creates a color-neutral appearance. Inner Shell: Aggregates are gradually added on site to achieve the correct consistency. The cellulose prevents the gravel from sinking during the curing period.

-Hydration retardant: It will leave visible the surface dispersals including a thin paste-like white cement concrete mix.

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Can fuel cell-catalysts be designed by simply counting nearest neighbors?

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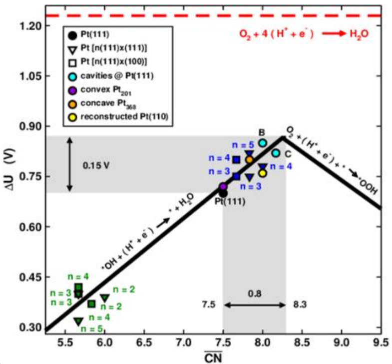

Figure 1: Coordination-activity plot for the ORR catalyzed by Pt-surfaces and its nanostructures. The plot correlates the GCN with the potentials of the ORR limiting steps. The ORR overpotential is the difference between the red line and those potentials.

In recent years, one of the main focuses of the car development industry has been on finding new and promising alternatives to combustion engines. Low temperature fuels cells could be a possible, environmentally friendly replacement. Their main drawback is that the best catalysts for the oxygen reduction reaction (ORR) consist of expensive platinum. Hence the catalyst activity must be optimized. Among simple platinum surfaces the (111) facet shows the highest activity for the ORR.

Interestingly, its performance can further be enhanced by the introduction of steps or concave defects. However, the origin of this higher activity of state-of-the-art catalysts with defects has not been properly explained.

Regarding the understanding of the exact reaction mechanism, predictions for the activities of newly designed surfaces are normally based on time-consuming density functional theory (DFT) calculations. However, this method is not suitable for screening a large array of surfaces. Faster methods could be developed by understanding the properties of the active sites responsible for the electrochemical reduction of oxygen. In this context, generalized coordination numbers ($\overline{CN}$) offer a simple solution.

$\overline{CN}$ is a geometric descriptor, which links the activity for the oxygen electroreduction with the geometry of the potential active sites by taking into account the coordination numbers of its neighboring atoms.

Plotting $\overline{CN}$ against the activity of already studied surfaces demonstrates its predictive power. The so called coordination-activity plot allows estimating the activity of potential catalysts for a specific reaction in a short timeframe. Calculations and experimental data show that the optimal value for the generalized coordination number should be approximately 8.3 for the ORR on platinum (see Figure 1).

In contrast, the $\overline{CN}$ of Pt(111) is only 7.5. Introducing either three or four atom wide (111)x(111) terraces increases the value of platinum already towards 7.83 and 8.0, respectively. This is in good agreement with our experimental finding that Pt(221) is the most active surface, even more active than Pt(331), the previously assumed most active Pt surface.

A similar effect can be observed on platinum nanoparticles. On a convex particle the activity is mostly determined by the surface area consisting of (111) facets. There are several potential approaches to increase their activity: Either the particle has to be specifically designed in a complex manner or several nanoparticles need to come into close contact and form more sophisticated structures. In both cases, active sites with a higher $\overline{CN}$ are formed, which increases the activity (see Figure 2).

These findings offer the possibility to design economically viable catalysts for the oxygen electroreduction, which in turn will ensure a green future mobility.

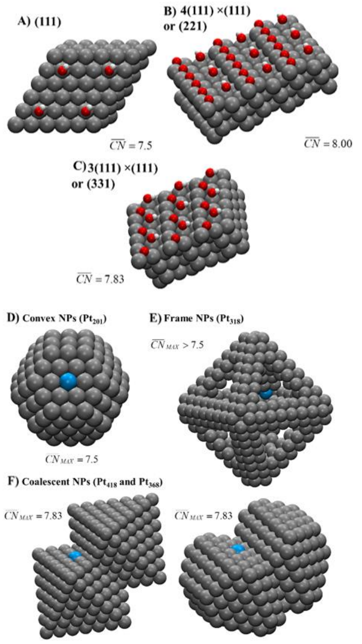

Figure 2: Most active sites on various Pt nanostructures. The sites with the largest and nearly optimal *OH adsorption energies appear in blue/red. The single red balls represent irreversible absorbed oxygen.

Investigating the structural changes in hybrid organometallic lead halide perovskites

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Growing global energy demand, driven by population growth and rising standards of living in developing countries, suggests a global appetite for energy in 2050 roughly double that of today and perhaps the most viable solution to the increasing demands is by harnessing the potential of natural energy sources. However, renewable energy projects require huge capital and so far have produced only small amount of world's energy consumption. Predictably, it will take almost a decade and some progressive steps so that renewable energy hold a major share in total energy output. Currently, the scenario is challenging as increasing cost of raw material, complex machinery and increasing cost of fossil fuels have slowed down the pace at which these renewable energy projects were to take off.

Over the past half a decade, organometallic lead halide perovskites have emerged as serious frontrunners as photoactive materials for sensitized solar cells, owing to the ease of manufacturing, abundance of materials and exceptional material physics with perovskite solar cells having reached a certified efficiency of 22.1%. The inception of perovskite solar cells goes back to a fortuitous experiment when a well- studied material [1, 2] was for the first time applied to the field of photovoltaics [3]. The term perovskite refers to a crystalline structure of solids. The deceivingly simple archetypal ABO¬3-type perovskites however have intriguing characteristics properties (magnetic behavior, high temperature superconductivity, ionic conductivity etc.) which may be attributed to the versatility of their structure and the transformational changes they undergo.

Compositional engineering of materials [4] has led to progressive development of optimized structures, but in spite of the steep growth curve of the incipient technology, the field is wrought with challenges of material structural instability and limited device lifetimes. The field poses numerous open questions regarding the intrinsic correlation between the crystalline structure of the material and the device performance which necessarily require to be disentangled before commercialization of this promising technology is feasible. We aim to analyze the issue by means of varying the compositional phases in a mixed hybrid perovskite, and following the subsequent structural changes by grazing-incidence wide angle X-ray scattering (GIWAXS)[5]. We plan to further correlate the structural information of the hybrid systems to the electronic properties of the material by characterizing solar cells. A more thorough understanding of the materials' attributes would go a long way towards the fabrication of long term stable and efficient solar cells.

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Following the Morphology Formation in Situ in Printed Active Layers for Organic Solar Cells

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Organic solar cells are a promising alternative to silicon based inorganic photovoltaic devices. Latter ones require a large amount of material and a high energy input for the production of the solar cell modules. This is a significant drawback for the inorganic devices in terms of environmentally friendly processing. Organic solar cells have the advantage that materials with very strong absorption can be used, reducing the overall needed amount of material for the active layer. Furthermore, another key advantage of organic photoactive layers is the possibility to process them out of solution. Using this property offers the opportunity to produce the active layer of the organic solar cell via printing methods and allows for up-scaling to industrial-oriented scales which is not the case for laboratory techniques like spin coating. Thus, roll-to-roll processing on flexible substrates is a production technique for organic solar cells we aim for. However, a lot of effort has to be spent on improving the functionality and thus efficiency of the printed devices. The inner film morphology has an enormous impact on the charge transport and therefore on the device performance. Tuning and influencing the assembly of the materials in the organic thin film on the nanoscale is still challenging and a better knowledge of the structural development is of utmost importance in order to successfully manipulate the inner film morphology. While there are investigations on the development of nanoscale morphology in polymer:fullerene photoactive layers during solvent casting, not much is known about the appropriate development in printed systems.

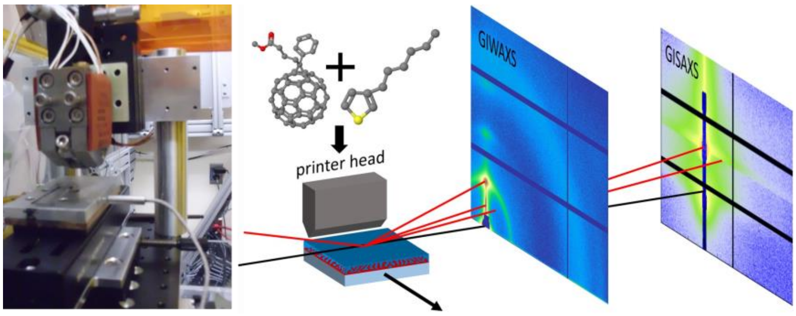

Figure 1: Photograph of the printer and sketch of the experimental setup

Useful techniques for investigating the inner morphology of a thin organic active layer are grazing incidence wide and small angle X-ray scattering (GIWAXS and GISAXS). These methods provide information about different length scales depending on the distance between sample and detector. An X-ray beam impinges the sample under a shallow angle to probe as much volume as possible and is scattered by the material depending on its crystallinity and assembly due to different electron densities. The scattered intensities are recorded on a 2D-detector and can be transformed to real space information. The setup and the detector patterns are shown in Figure 1. By implementing the printer into a synchrotron X-ray beam, we can watch the structure forming while printing (*in situ*). This way we obtain insight into the crystallization kinetics and structure formation of a slot-die coated polymer:fullerene active layer. Quantitatively analyzing the data, we are able to provide a model of the inner structure formation (Figure 2). This knowledge is important for further influencing the inner nanoscale morphology in printed films to optimize the device performance of organic solar cells in an up-scalable technique.

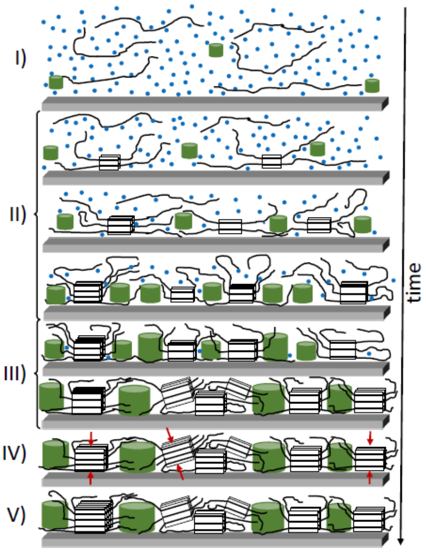

Figure 2: Model of structure formation

Reference: S. Pröller et al., Adv. Energy Mater., 6: 1501580 (2016)

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Investigation of carbon supported Ta- based nanometric compounds as ORR catalyst for PEMFC

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High cost and limited availability of platinum-based catalysts for Oxygen Reduction Reaction (ORR) is a major hurdle towards the commercialization of Proton Exchange Membrane Fuel Cell (PEMFC) systems. Until today, replacing Pt by Pt-free and finally by noble-metal-free catalysts for ORR is still restricted to the labs. High activity and durability are the main requirements for a new catalyst. MN_xC_y system (M = Fe, Co) are favored due to their low cost, reasonable activity and remarkable selectivity towards ORR[1]. On the other hand, MN_xC_y catalysts have a disadvantage in their poor stability in corrosive environment. Since more than a decade, Ota *et al.* are studying valve-metal oxides (from group IV and V) compounds[2], observing some ORR activity for those compounds. Additionally, they found that these metal oxides are stable in an acid solution. Based on their work, we started our research on the same system, starting with carbon-supported (Ketjenblack EA-type, KB_{Graph}) Ta-based compounds[3]. The samples were synthesized from a self-made air stable organometallic precursor namely, tantalum phthalocyanine trichloride ($TaPcCl_3$). Various synthesis conditions were used by changing the temperature and gas composition. Figure 1 shows the X-ray diffractograms of supported nanometric Ta-based compounds from the precursor. We found that for the samples synthesized at 1000 °C in 0.05% oxygen we have a mixture of tantalum carbide/carbonitride and orthorhombic tantalum pentoxide (Ta_2O_5). For samples synthesized at 600 and 700 °C we have only hexagonal Ta_2O_5. Furthermore, the ORR electrochemical activity of these samples were tested by thin-film RDE technique at 20 °C in 0.1 M $HClO_4$ electrolyte (Figure 2)[4]. Comparing the ORR results it is clearly seen that, in the synthesis-temperature at 600 °C, hexagonal Ta_2O_5 shows relatively higher activity than others. For the future it would be interesting to investigate the correlation between structure of Ta_2O_5 and ORR-activity. Further, doping by aliovalent cation could also be an interesting route to increase the ORR-activity.

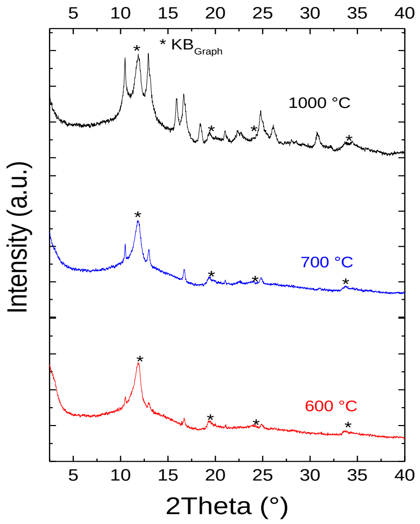

Figure 1: X-ray diffractograms of carbon supported Ta-based compounds synthesized at different temperatures

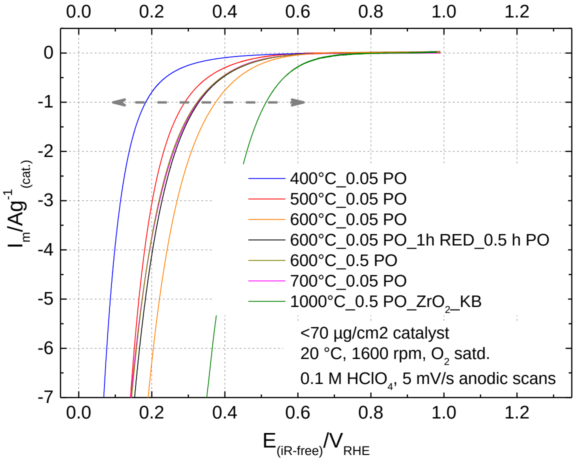

Figure 2: Difference in ORR mass activities of synthesized Ta-based compounds

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Positrons Revealing Lattice Defects in Energy Materials – Functionality of Thin YBCO Films

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Many novel concepts in energy science are based on new and complex materials with exceptional functionalities. In their practical application lattice defects often play a key role because they are either disadvantageous or favorable for technical application. Exemplary, in solar cells defects reduce the efficiency whereas in ion cell materials vacancies and grain boundaries accelerate atomic diffusion processes during charge-discharge circles. In order to probe the presence of vacancies down to a concentration of 10^{-7} per atom we apply Positron Annihilation Spectroscopy (PAS). The positron as probe particle exhibits an outstanding sensitivity on any kind of open volume defects. The use of the high intensity positron beam NEPOMUC at the FRM II even allows imaging the 3D distribution of such defects.

We investigated the high temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) as most prominent representative of the wide class of superconducting cuprates. Due to its high critical temperature T_c of 90 K YBCO is already technically used in superconducting wires, magnets and fault current limiters. Superconductivity in this system seems to be intertwined with charge-density-wave order from which a variety of exotic physical phenomena emerge. A decisive parameter in technical applications and fundamental research is the oxygen deficiency δ. Within the last decades the progress in pulsed laser deposition made the controlled growth of single crystalline YBCO films of unprecedented quality feasible. Due to the limited thickness of several 100 nm of such high-quality YBCO films the determination of δ and in particular its spatial distribution remains challenging. We have established PAS at the NEPOMUC positron beam as new experimental tool for revealing the 3D distribution of oxygen atoms. This distribution was found to depend on atomic diffusion processes during the complex preparation of the samples which determine δ.

We evaluated the spatial variation of δ [1,2]. The lateral variation and the depth dependency of δ have to be considered separately. Atomic diffusion processes during the film production are driven by exchange of oxygen atoms at the surface and the interface to the substrate. In thermal equilibrium lateral inhomogenities are expected to vanish whereas a pronounced depth dependency of δ was observed leading to a depth dependent critical temperature T_c. We assume that due to a very high δ superconductivity vanishes close to the surface while it prevails close to the interface at maximal T_c. These results demonstrate that further optimizing preparation processes of YBCO films have great potential to significantly improve the performance of superconducting devices.

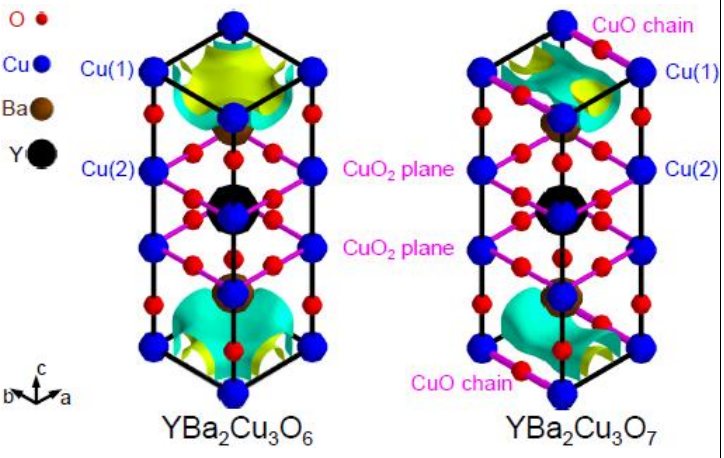

Figure 1: Isosurface of the positron density in insulating $YBa_2Cu_3O_6$ and superconducting $YBa_2Cu_3O_7$

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Development and Assessment of a Cradle to Cradle® inspired Plus-Energy-Home

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Considering the global challenge of scarcity of resources, the construction industry plays a key role. Therefore, we have to fundamentally reconsider the use of resources such as energy, materials, water, etc. for construction, operation and dismantling of buildings.

The Cradle to Cradle philosophy challenges existing building concepts with a holistic view of the building life cycles to achieve a fundamentally positive footprint. The University of Texas at Austin (UTA) and the Technische Universität München (TUM) developed, designed and built the so-called “nexushaus” as part of the international competition “Solar Decathlon 2015” organized by the U.S. Department of Energy. Based on three design criteria of Cradle to Cradle (C2C): “Waste equals food”, “Use current solar income” and “Celebrate diversity”, the two universities implemented related ideas into their building concept. After the Solar Decathlon competition, the present research project is now evaluating the experiences, gained during the whole planning process of the nexushaus. Final goal of the research project is the development of a guideline on how to implement the C2C principles into the building environment. Thus, the following goals are representing the core elements of the guidance:

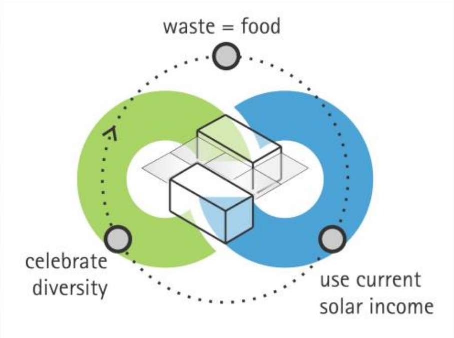

Figure 1: Implementation of the C2C design criteria in the building sector.

“Waste equals food”

The materials used for the building construction will be delivered from sustainable sources and local manufacturers to minimize the embodied energy. To ensure a high quality of interior comfort for the users, the building components should be selected without pollutant ingredients and free of volatile organic components (VOCs). Every material is defined as biological and/or technical nutrient. After end of life, the product components, as technical nutrients, will be re-used and recycled by the manufacturer, in order to create new building products. Within the biological cycle material, e.g. untreated wood, could be composted and could serve as a nutrient for natural processes.

Integrated closed water cycles reduce the amount of potable water provided by the public infrastructure. Rainwater will be captured and filtered in order to provide potable water for the house. The Greywater of shower, sink and washing machine is used for garden irrigation. Evaporated water from the air-units will be forward to the fish tank of an aquaponic-system, which is an innovative concept providing a closed water loop that irrigates crops for food production.

“Use current solar income”

Within the life cycle of the house, more energy will be produced than consumed. Besides that, the surplus generated power will charge an electric car. By zoning the house into day and night modules, the user is able to control which module is using more electricity, such as air conditioning or lighting, throughout the day/night.

“Celebrate diversity”

As a cost-efficient solution the house adds density to located neighborhoods without requiring additional infrastructure through the utilization of the city. The modularity allows flexibility to different property sizes and adaptability to user changes. The installed SmartHome-System visualizes the impact of occupant behaviour on energy and water consumption.

To address the related social, environmental and economic challenges of today an integrated, holistic approach has to be taken to achieve buildings with a positive footprint. The nexushaus is the first prototype of the Cradle to Cradle philosophy and provides a base for future, sustainable construction methods.

Hybrid thermoelectrics based on a polymer/nanoparticle composite

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The usage of fossil fuels has led to increased levels of greenhouse gases, which in turn result in devastating meteorological phenomena. Indications of this imminent change in global climate have, over the past years, been responsible for an increased interest in techniques for power generation based on renewable energies.

Solar cells possess the ability to convert visible solar radiation into electrical power. While they are already highly efficient and have been implemented in daily life, it is also feasible to think of alternative ways of harvesting energy. Heat is lost in almost all processes which occur in daily life, which is evident looking at the heat production in the human body or in combustion engines in cars. It is desirable to transform this low-quality form of energy into high-quality energy in the form of electrical power.

Thermoelectric materials are able to generate an electrical voltage upon application of a temperature gradient along the material. The gradient leads to a flow of charge carriers from the hot to the cold side and therefore to an imbalance in the charge distribution. The occurring thermovoltage or Seebeck coefficient (S), along with electrical (σ) and thermal conductivity (κ) can be put into the following equation for the temperature-dependent figure of merit ZT, which directly correlates to the energy conversion efficiency at a given average temperature: $ZT = (\sigma S^2/\kappa)T$.

Although inorganic thermoelectrics based on elements such as Te, Se, Pb, Bi, As, etc., exhibit high values for ZT, the price, low abundance, potential toxicity and environmental concerns regarding the raw materials have impeded the large-scale application for heat conversion.

Using the electrically conducting polymer blend PEDOT:PSS, we want to overcome the limitations of inorganic thermoelectrics, by making use of the high abundance of raw materials, facile solution-based processing and lowered toxicity. In literature, many different procedures for improving the electrical conductivity, usually by treating thin films with high-boiling solvents or other chemical agents, have been shown [1].

In our approach, we wish to tune the thermoelectric parameters, especially the thermal conductivity, by means of nanostructuring using inorganic nanoparticles. While maintaining a high electrical conductivity it should reduce the thermal conductivity through phonon scattering. We are able to fully characterize the polymer films regarding their thermoelectric properties, by using standard techniques for determination of S and σ and IR thermography for determination of κ. This enables to calculate ZT values for PEDOT:PSS thin films. In addition, we performed tender resonant x-ray scattering (T-ReXS) experiments on the PEDOT:PSS/Si-NP composite films using synchrotron radiation energies close to the sulfur K-edge. Using the contrast variation capabilities of this technique, we are able to devise a structural model and attempt to correlate this with the thermoelectric properties of the composite films.

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Organic-inorganic hybrid membranes for lithium–ion batteries

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In the light of an increasing demand on power sources for portable electronic devices, the nano-scaled lithium based membranes paves the way for new opportunities regarding design, application and integration of rechargeable batteries.

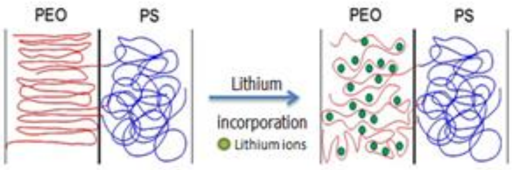

Figure 1: Schematic illustration of lithium salt incorporation in PS-*b*-PEO diblock copolymer

In this work, the morphology and conductivity of a high molecular weight polystyrene-*block*-polyethylene oxide (PS-*b*-PEO) block copolymer containing lithium salt and titania nanoparticles were investigated at different temperatures. The crystallization of the PEO block was highly suppressed at a certain Li-salt doping level as well as upon increasing titania concentration. The small-angle X-ray scattering (SAXS) measurements indicated a morphological transition from lamella to cylinders and spheres with subsequent solid-state hybrid membrane amorphisation.

An enhanced ionic conductivity is found to be correlated to the enhanced microphase separation of the lithium containing polymer. The correlation between the morphology and ionic conductivity of the lithium containing block copolymer electrolytes provides an insight into the mechanisms responsible for the conduction of lithium ions in these systems. A proper amount of titania nanoparticles suppresses also the dendrite growth of the battery electrodes and therefor enhances the cycling stability of the cell.

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Morphology and crystal orientation of hybrid perovskite thin films for photovoltaic application

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Organo-metal halide perovskites mark a paradigm shift in photovoltaic research, as they combine high power conversion efficiencies (PCE) with easy processing and cheap abundant precursor materials. Recent reports of PCE crossing the 20% mark are possible due to remarkable material properties and their highly crystalline nature even when processed from solution. Thus, in only about five years of research this new class of hybrid materials has become a promising contender for other inorganic thin-film photovoltaic technologies or even commercially available monocrystalline silicon solar cells. The commercial application of perovskite solar cells, however, is so far impeded by fundamental understanding lacking behind this fast progress in device efficiency. The most challenging questions tackled by scientists are the origin of a hysteresis frequently observed in current-voltage characterization and the reproducibility of devices, both of which are strongly linked to film morphology which in turn depends on the applied preparation protocol. We investigated hybrid perovskite thin films of high efficiency solar cells prepared by various synthesis protocols with grazing-incidence wide angle X-ray scattering (GIWAXS) which revealed dramatic differences in crystal orientation. Thereby, we evidence that different crystallization mechanisms lead to certain morphologies and crystal orientations reflecting the chosen synthesis method [1]. Especially one method was studied in detail as it interestingly showed both of the two preferential orientations that can be present in perovskite films. This method is an established 2-step synthesis that has led to highly efficient solar cells [2]. It comprises the deposition of a precursor layer (PbI_2) from solution by spin-coating and the subsequent conversion to perovskite by dipping into a mixed solution of methylammonium halide salts (MAI and MACl).

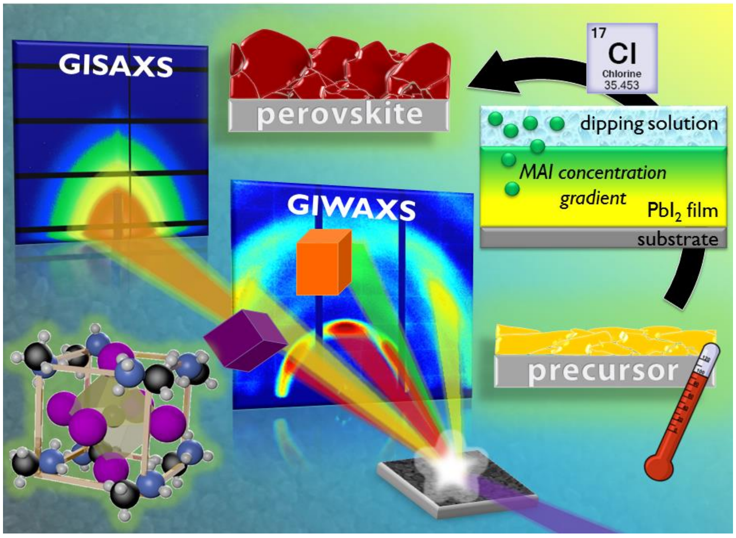

Figure 1: Schematic summary of the investigations on perovskite conversion mechanism.

We have investigated the precursor and resulting perovskite with grazing incidence small angle X-ray scattering (GISAXS). We observe a strong correlation of lateral crystal sizes before and after conversion which we attribute to constrained crystal growth. Additionally, we find an accumulation of smaller crystals within the film in contrast to the surface which reveals laterally differing conversion processes: While the higher concentration of ions inside the dipping solution leads to Ostwald-type ripening on the film surface and large crystals are formed, large crystals inside the film crack up due to spatial confinement [3]. Together with our findings from GIWAXS measurements, we conclude that up to three competing conversion mechanisms are present which are linked to certain crystal orientations. The preference of each mechanism is tunable by the processing parameters like temperature and ion concentration or species. Thus, our results mark an important step towards a rational development of new synthesis methods for high efficiency perovskite solar cells.

[1] L. Oesinghaus *et al.* (in preparation); [2] P. Docampo *et al.*, Adv. Energy Mater. 4 (2014) 1400355;
[3] J.Schlipf *et al.*, J. Phys. Chem. Lett. 6 (2015) 1265–1269.

Highly ordered titania films for application in perovskite solar cells

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As the need for renewable and sustainable energy increases, the investigation and development of renewable and sustainable energy sources is an important field of research. Among the most promising developments are perovskite solar cells, the best of which yield high efficiencies of up to 20,8%, employing simple production techniques and abundant materials. A high demand for easily producible perovskite solar cells is to be expected in the future as this technology is likely to have lower cost than silicon photovoltaic modules jointly with a high performance.

Photovoltaic applications benefit from the remarkable electronic and optical properties of perovskite absorber layers that derive from the perovskite lattice structure. Metal halide perovskites of the structure ABX_3 display the same crystal structure as calcium titanate, in which A and B denote cations, coordinating with 12 and 6 anions X, forming cuboctahedral and octahedral geometries respectively. Until now, the most successful perovskites for photovoltaic applications are $CH_3NH_3PbX_3$ (X = Cl, Br, I) compounds, due to their strong absorption, high charge carrier mobilities and diffusion lengths.

In principle, perovskite solar cells have the same device architecture as dye-sensitized solar cells, which can be described, in the most general way, as an absorbing layer stuck between an electron- and a hole-transporting layer. Upon illumination, excitons are generated in the absorbing layer and extracted by the respective transporting layers. The properties of perovskite solar cells are known to be sensitive on the various processing conditions, such as the material ratios and atmospheric conditions, which strongly affect the film quality of the perovskite and therefore the device performance.

Within this work, we focus on the deposition of perovskite on highly ordered mesoporous titania films. The orientation of the crystalline perovskite as function of the titania film morphology, the carrier recombination and the cell performance are studied. The morphology of the mesoporous titania and of the perovskite films is characterized by SEM and AFM. The crystal phase and optical properties of the perovskite are probed with X-ray diffraction and UV-Vis spectroscopy, respectively.

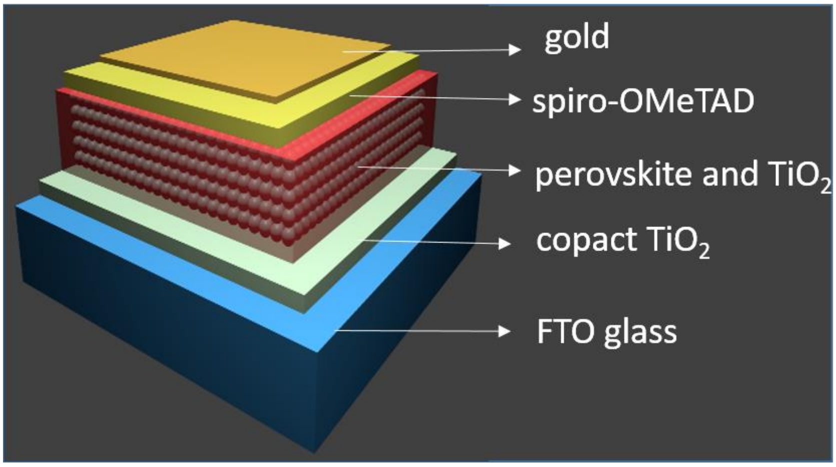

Figure1: Architecture of a perovskite solar cell

Influence of processing parameters on the morphology of perovskite solar cells

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Over the last decade, alternative materials for photovoltaic solar cells came into focus of many research groups around the world. Especially lead halide perovskites as an organic-inorganic hybrid compound received attention due to the exceptional rise in the power conversion efficiency (PCE) of research cells from 3.8 % in 2009 to 22.1 % in early 2016 [1]. This vast increase efficiency creates the demand for easily producible perovskite solar cells for commercial purposes as this technology promises low production cost compared to e.g. silicon photovoltaics.

The most common active layer perovskite material is methylammonium lead iodide ($MAPbI_3$). As an absorber layer in photovoltaic devices it offers a PCE similar to prevalent thin film and silicon solar cells. The abundancy of all compounds applied in these cells combined with the possibility of solution processing or spray deposition promises a simple and also cheap production.

The good performance is caused by the special properties of $MAPbI_3$ like a high intrinsic absorption, high open circuit voltage and ambipolar electron and hole transport with large diffusion lengths.

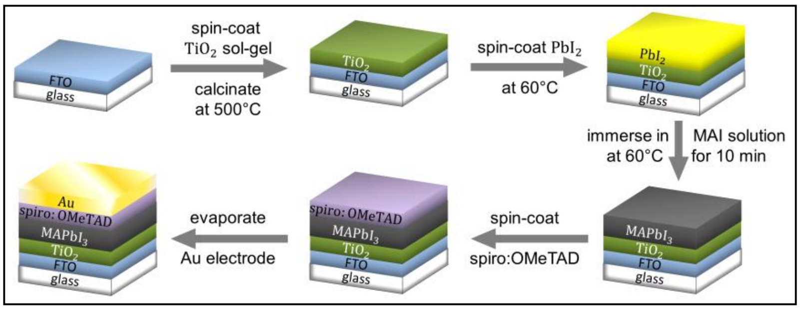

Figure 1: Solution conversion solar cell preparation routine

Despite the interest in perovskite containing solar cells has risen throughout the last years, there are still some open questions for basic research. One of those issues is the origin of the hysteresis observed in the I-V-characterization and the resulting ambiguity of determined PCE.

Figure 1 shows a common process for the fabrication of planar perovskite solar cells, in which a PbI_2 layer is deposited by spin coating at 60 °C and subsequently immersed into a solution of MAI at 60 °C for a specific time [3]. This leads to strong preferential crystal orientations as evidenced by grazing-incidence small angle X-ray scattering (GIWAXS) measurements. The crystal orientation is tunable via temperature variation of precursors of the perovskite and the use of additives into the precursor or conversion solution [2]. This is due to fundamentally different crystallization processes that are influenced by the choice of processing parameters like the immersion time into the conversion solution. In the present work, we expand this study by the use of mixed solvent approaches with processing additives in order to further tune the time scales of the crystallization processes and gain more control of the film morphologies of perovskite thin films.

Ultimately, controlled thin film morphologies are crucial for the commercial application of highly efficient perovskite solar cells.

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NMR parameter computations and the electronic structure of oxygen-deficient LTO

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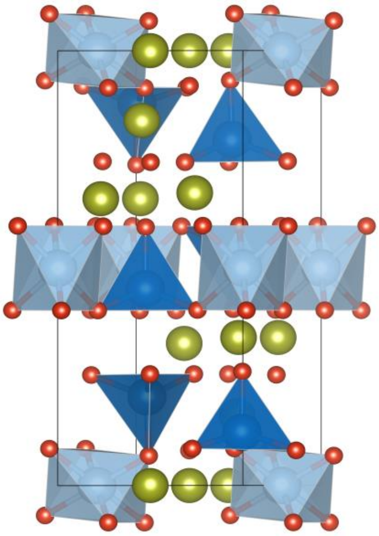

Figure 1: LTO crystal structure

Spinel-structured lithium titanium oxide $Li_4Ti_5O_{12}$ (LTO) is a promising zero-strain anode material for rechargeable lithium ion-batteries addressing safety and durability issues persisting for carbon-based anodes. Its relatively low electronic conductivity can be improved by introducing oxygen vacancies [1].

Experimental XPS [1] and EPR [2] results suggest the partial reduction of Ti ions. The description of the respective mixed-valent transition metal cation distribution is challenging for DFT methods. LTO's inherent stoichiometric disorder and the spatial separation of vacancies from periodic images additionally requires large supercells.

We have conducted systematic studies employing PBE, DFT+*U*, and hybrid functionals. The expected gap states are found with all methods. However, the spacing between those localized states and the valance band minimum is not described properly by the PBE functional. To obtain more reliable results (compared to PBE) with less computational cost (compared to hybrid functionals) a suitable *U*-parameter is determined.

Computed quadrupolar coupling constants for Li NMR spectroscopy are correlated with local geometric distortions and the electronic structure in the vicinity of O–vacancies, allowing for future combined theoretical and experimental NMR studies of the microscopic ion transfer pathways in this interesting material.

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Characterization of CO_2 methanation catalysts

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Recently, CO_2 hydrogenation to methane regained the interest of researchers as a promising storage technology for renewable energy. Among several catalysts for CO_2 methanation, supported Ni is the most widely investigated. A key factor in catalytic performance is the metal dispersion and the metal surface area. This contribution presents the synthesis of highly dispersed Ni/SiO_2 and Ni/Al_2O_3 catalysts with a high metal surface area. Next to standard methods, selected catalyst samples are characterized via H_2-TPD and N_2O chemisorption, the latter of which Tada et al. recently applied to characterization of Ni catalysts successfully for the first time [1]. Samples studied by Tada et al. were impregnated $Ni/\alpha\text{-}Al_2O_3$ catalysts.

The Ni/Al_2O_3 catalyst with a Ni loading of approximately 40 wt% was synthesized via coprecipitation of the corresponding metal nitrate salts followed by calcination [2]. Static H_2 chemisorption gives a Ni surface area of 17.1 $m^2/g_{cat.}$ The highly dispersed Ni/SiO_2 catalysts were prepared by means of the chemical vapor deposition in a fluidized bed reactor consisting of a quartz reactor, a saturator and an oven. For the deposition, a volatile metalorganic nickel precursor is used and the deposition was conducted by lowered pressures and elevated temperature. The screening of the activity was done in a single-pass tubular reactor where the methanation performance was determined by measuring the CO_2 conversion at different temperatures. Metal dispersion of different Ni/SiO_2 catalysts synthesized by means of the chemical vapor deposition are shown in Figure 1. As it can be seen, the dispersion increases with increasing nickel loading in the range between 0 to 5 wt%. If the nickel loading reaches 6 wt%, the dispersion starts to spread around a value of 30 %. With specific posttreatment parameters during the calcination of the catalysts, it is also possible to increase dispersion up to 45 %. A very high dispersion of these catalysts also indicate that the overall H_2 uptake is equal or higher as the pristine Ni/Al.

H_2-TPD and N_2O chemisorption experiments with the coprecipitated Ni/Al_2O_3 catalyst and a 12 wt% Ni/SiO_2 catalyst synthesized by CVD were conducted in a flow-setup equipped with a quadrupole mass spectrometer. Results are depicted in Figure 2 and 3. Prior to TPD, H_2 was adsorbed using a continuous H_2 stream or by applying 40 pulses of diluted H_2 so that a breakthrough of H_2 could be detected. N_2O chemisorption was conducted as a flow or titration experiment. In the case of Ni/Al_2O_3 the Ni surface area of 16.6 m^2/g_{cat} after pulsed H_2 adsorption agrees well with results from static H_2 chemisorption. The Ni surface area is 24.6 m^2/g_{cat} when adsorbing H_2 for 30 min. Mild conditions are required when conducting H_2-TPD for Ni surface area determination. N_2O chemisorption as well as N_2O titration (not shown here) give a significantly higher Ni surface area. In contrast, N_2O chemisorption with the Ni/SiO_2 catalyst gives a Ni surface area of 31.3 $m^2/g_{cat,}$ which is in accordance with 29.1 m^2/g_{cat} from static H_2 chemisorption. N_2O chemisorption is capable of determining the metal surface area of SiO_2 supported Ni but seems to overestimate the Ni surface area of the precipitated Ni/Al_2O_3 system. To what extent the synthesis procedure and catalyst support influence N_2O chemisorption is currently under investigation.

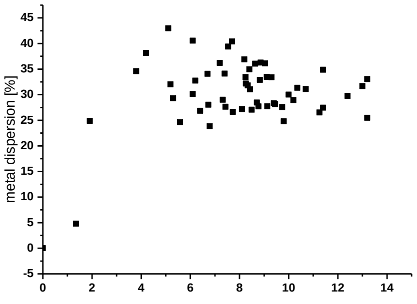

Figure 1: metal dispersion vs nickel loadings of highly dispersed Ni/SiO_2.

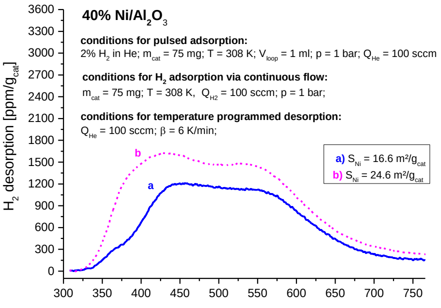

Figure 2: TPD after H_2 pulse adsorption (curve a) and adsorption for 30 min (curve b).

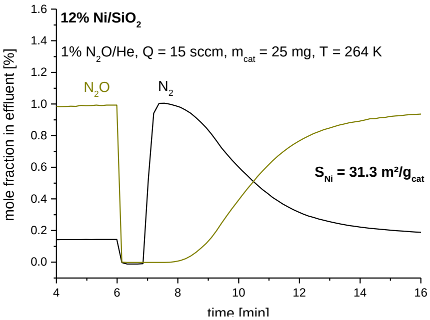

Figure 3: N_2O Chemisorption result with Ni/SiO_2.

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Degradation effects of high efficiency polymer solar cells

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Presently, about two thirds of electricity consumed on earth is derived from burning fossil fuels such as coal, oil and natural gas. However, their availability is limited and the main burning product CO_2 leads to an enhanced greenhouse effect. These challenges can only be faced with a reorientation towards renewable energy sources. Solar cells give us the opportunity to use the radiation energy of the biggest renewable energy source, the sun, to directly generate electricity.

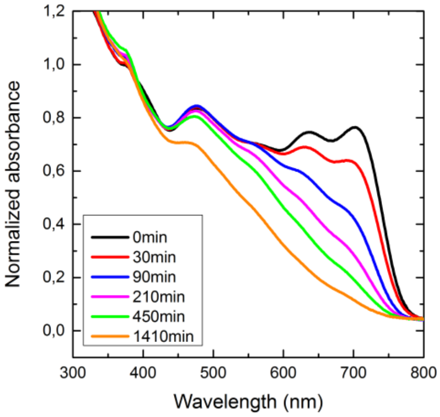

Figure 1: UV/Vis spectrum of the active layer of an organic solar cell

Today industrially used solar cells are mainly based on silicon technology. With this technology, power conversion efficiencies of over 25% [1] can be reached and they have a life time of a few centuries. But there is also a drawback, as the production of silicon solar cells is very expensive and energy consuming. An interesting alternative for silicon are organic materials. The application of polymers as active material has several advantages. They are typically cheap in production, flexible and lightweight, but their efficiencies and long-term stabilities are far below the ones of silicon. In the last years, research has been focusing on the identification of new high-efficiency polymers. These new polymers have smaller band gaps leading to an increased photon absorption. Examples are PTB7 and its derivatives with which power conversion efficiencies of over 10% [2] can be achieved. However little is known about the long-term stability of these polymers, but for a profitable large-scale production the lifetime is an important parameter.

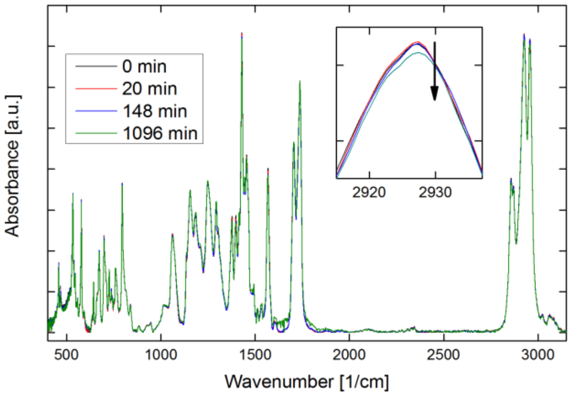

Figure 2: FT-IR absorption spectrum of active layer films measured at different illumination times, enlarged CH2 asymmetrical stretching peak

In particular degradation effects under UV irradiation are of interest. Therefore, the samples were illuminated with UV and visible light under ambient conditions and measurements were taken out after different illumination times. In figure 1, the UV/Vis absorbance spectra of an active layer with a high-efficiency polymer are plotted. At longer wavelengths, a fast decrease of the absorbance due to the bleaching of the polymer can be seen. Degradation processes in organic solar cells can be split into chemical processes, like photo-oxidation or photo-bleaching, and physical processes caused by morphological changes. Changes in the molecular structure of the polymer can be investigated by analyzing the infrared absorption spectrum of the used active material. In figure 2 the results of such a measurement for active layer films can be seen. In the figure inlet one peak (CH_2) is shown in more detail. The absorption of this peak decreases with time, meaning that some of the CH_2-bonds are broken. In further investigations we concentrate on at different methods to prevent degradation in this low bandgap polymer.

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Single-Solvent Electrolytes for Lithium-Ion Batteries Studied by *Operando* Diffusive Reflectance Infrared Fourier Transform Spectroscopy

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In battery research, there is a big interest in surface characterization techniques such as X-ray photoelectron spectroscopy (XPS) or infrared spectroscopy (IR) in order to characterize the electrode decomposition products on the electrode surface. At the same time, gassing phenomena are characteristic for electrolyte decomposition processes [1, 2], whereby on-line gas analysis can provide insight into the corresponding reaction mechanisms [3, 4].

In the present work, we developed a novel cell design for *operando* Diffusive Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS). Using this setup, the working electrode is monitored spectroscopically during electrochemical cycling. Compared to the setup described in the literature [5, 6], our *operando* DRIFTS has two major advantages. First, with our cell we do not only observe the electrode surface and electrolyte, but also gas evolution during electrochemical cycling. Second, for our DRIFTS studies we use half-cell stacks with separator and working electrode materials that are closer to commercial batteries than the setup described in the literature.

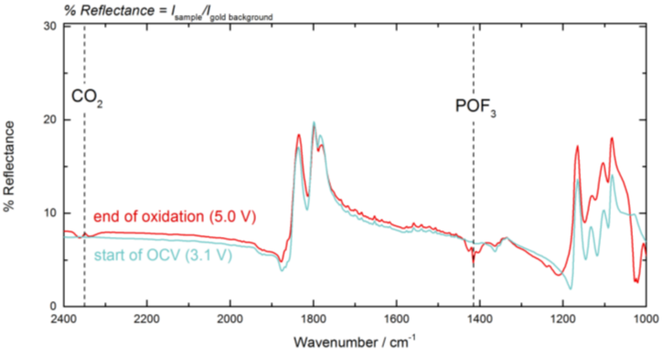

Figure 1: *Operando* DRIFTS data of an LFP half-cell with 1.5 M $LiPF_6$ in pure vinylene carbonate before and after oxidation to 5.0 V. The spectra show distinct signals of the gases CO_2 and POF_3 after the oxidation process.

Operando measurements were performed with lithium half-cells. To facilitate spectral interpretation, single solvent electrolytes such as solutions of $LiPF_6$ in pure ethylene carbonate (EC) or vinylene carbonate (VC) were applied. Inside our setup, the infrared radiation is diffusively scattered at the working electrode surface. We chose materials such as $LiFePO_4$ and $Li_5Ti_4O_{12}$ for electrode preparation. Due to the fact that the infrared beam penetrates the gas volume in the head space of the cell, formation of gases is detected as well. For instance, we were able to detect gaseous POF_3 and CO_2 evolution during electrolyte oxidation at high potentials (see Figure 1). We will present EC and VC oxidation and reduction studies using *operando* DRIFTS.

Acknowledgements:

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Improvement of Mass Transport in Polymer Electrolyte Fuel Cells by Diffusion Medium Modifications

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Polymer electrolyte membrane fuel cells (PEMFC) are believed to play an important role in the growing field of electric mobility. These electrochemical devices convert the chemical energy of hydrogen into electrical energy by the reaction with oxygen to form water. This process is composed out of two reaction sequences which take place on different electrodes. One key component of PEMFCs is the diffusion medium (DM) which is used to homogeneously distribute reactant gases over the electrode surface, to efficiently remove product water, and to provide good electrical and thermal contact.[1] At high current densities, the formation of liquid water in the GDL can substantially impede oxygen transport and thus fuel cell performance.

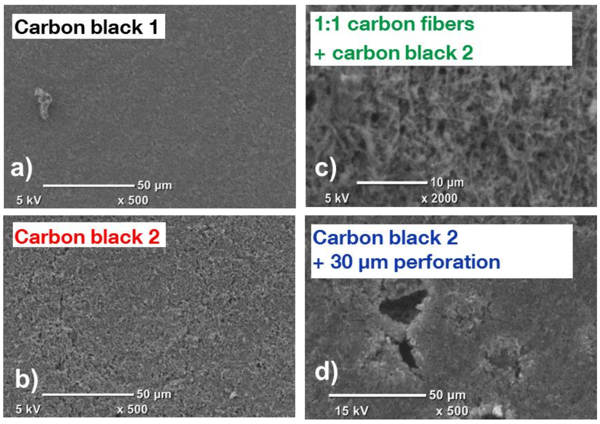

Figure 1: Scanning electron microscopy images of different microporous layer variations in top view.

Typically, the DM consists of a carbon fiber gas diffusion layer (GDL), which is coated with a microporous layer (MPL) in order to provide an intense contact between the large pores of the substrate and the small pores of the electrode. The MPL is a crucial component for the liquid water management of the fuel cell. On the one hand, it has to retain water at dry operating conditions to keep the proton conducting membrane humidified. On the other hand, at wet operating conditions, liquid water has to be removed from the electrodes to the gas flow channels. Conventional MPLs consist of carbon particles (e.g. carbon black or graphite) and PTFE as binder and hydrophobic agent (cf. Fig. 1 a/b). Especially liquid water transport is very sensitive to the porous structure. For example, it was observed that cracks act as transport pathways through the MPL.[2]

In this contribution we demonstrate the influence of water and oxygen transport on the electrical power of a single fuel cell. Specifically, by varying the type of carbon and perforation of the MPL (cf. Fig. 1), the transport of liquid water can be significantly enhanced. By using a different carbon black, we could reach a significant performance enhancement of a PEMFC operated under wet conditions (cf. Fig. 2). While we have not found improvement by blending carbon black 2 with vapor grown carbon fibers, artificially introducing pores within the MPL could increase the maximum current density by ~30% compared to carbon 1. This is attributed to an enhanced two-phase transport of water and oxygen.

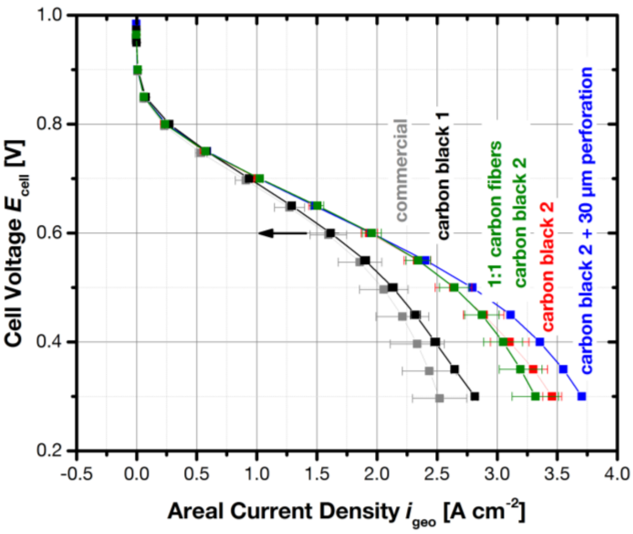

Figure 2: Fuel cell performance curves for different cathode microporous layer coatings. 5 cm² active area single cell test at 50 °C, 200 kPa_{abs} relative humidity of 120% and differential flow conditions.

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A low temperature route towards hierarchically structured titania films for thin hybrid solar cells

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Fabricating titania based solar cells at low temperature has a potential for energy-saving and for realizing flexible photovoltaic devices, since still most of the photovoltaic devices based on titania require high-temperature steps. Moreover, dye-free hybrid solar cells represent a novel approach, which lowers production costs and avoids problems related with dye bleaching. Therefore, dye-free hybrid solar cells are a promising alternative for current dye-sensitized solar cells technology.

Although many efforts have been made for boosting the photovoltaic performance of the dye-free hybrid solar cells, to date, most power conversion efficiencies (PCE) are generally less than 1 % even with high-temperature sintered titania films. In order to improve light harvesting in the active layer of the hybrid solar cells, we superimpose superstructures (micro-scale) on mesoporous titania films in the present work. The mesoporous titania films could be achieved via various routes, among which the sol-gel synthesis in combination with block copolymer assisted templating is very promising. In this approach, the morphologies of titania are controllable (ranging from form-like structure to worm-like aggregates by adjusting the reactant ratio in the sol-gel chemistry) and the mesopores can be tuned through the micro-phase separation of diblock copolymer induced by a so-called good-poor solvent pair. However, the sol-gel process normally results in amorphous TiO_2 rather than the crystalline phase which is required for the photovoltaic application. Therefore, we use a special titania precursor, ethylene glycol-modified titanate (EGMT), which could crystallize titania during the sol-gel process at room temperature. Afterwards, the resulting films are patterned by nano-imprint lithography (NIL) to achieve superstructures. In this study, we use a PDMS master for nano-imprinting. It features nano-pillars with size of 200×200 nm^2 and a lattice period of 400 nm as sketched in Figure 1. UV irradiation, is chosen to remove polymer template to obtain mesopores titania films. The surface and inner morphologies of the hierarchical titania film are probed by scanning electron microscopy (SEM) and grazing incidence small-angle x-ray scattering (GISAXS). The results show that the NIL does not impact titania nanostructures and mesopores establisged via sol-gel synthesis.

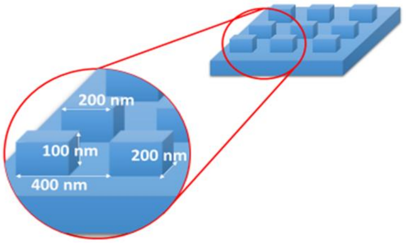

Figure 1: PDMS master for NIL

The achieved hierarchical titania films are backfilled with P3HT (exciton generator and p-type conductor).to realize the active layer. Next, the samples were post-annealed in nitrogen atmosphere at 120 °C for 10 min. The surface and inner morphologies of the active layer are also investigated with SEM and GISAXS measurements, respectively. The result indicates that P3HT could only infiltrate the large pores efficiently. The potential for light harvesting is characterized by UV-Vis absorption spectra, which suggests that the active layer with the hierarchical titania film can absorb more light.

Finally, we produce dye-free solar cells based on the hierarchical titania film at low temperature. From the current-voltage characteristics, the device with superstructured features exhibits better photovoltaic performance (Figure 2).

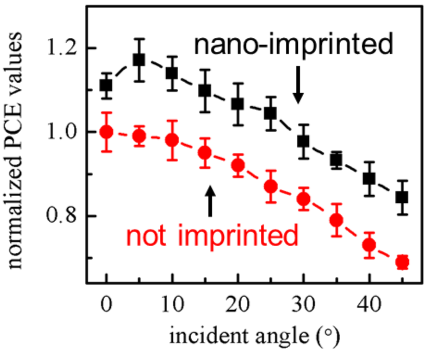

Figure 2: angular dependent PCE

Morphology of block copolymer electrolytes for rechargeable lithium-ion batteries

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Lithium-ion battery is one of the most promising energy storage systems. The Li-ion batteries have no “memory-effect” and have much higher energy density compared to other battery types. For instance, a Li-ion battery can store 3-4 times more energy than a Nickel-Cadmium battery. In standard Li-ion batteries, the electrolyte is fluid, which brings in fact a high ionic conductivity as an advantage. But this advantage comes with some disadvantages, like the danger of flammability or the possibility of short cuts through the formation of so called dendrites. These disadvantages are bypassed with the use of solid-state membranes as electrolytes.

Block copolymers (BC) electrolytes have been recently investigated as solid-state membranes for lithium-ion batteries [1]. Nanostructured BC electrolyte contains both, the ionic conducting as well as the high-tensile polymer domains, enabling both, high ionic conductivity and improved mechanical stability. Since the diffusion path of the Li-ions only follows the percolation path of the ionic conducting domain, the morphology of the BC electrolyte is an essential parameter.

Theoretical studies have recently reported that the BC electrolyte phase diagrams significantly deviate from the conventional BC phase diagrams due to electrostatic interactions between polar chains and alkali metal-ions [2]. This effect could be used to tune the morphology, thus optimizing the path for the migrating ions. The morphology of polylauryl methacrylate-*block*-polymethacrylic acid (PLMA-*b*-PMAA) diblock copolymer (DBC) electrolyte with two different ionic block volume fractions was investigated using scanning electron microscopy (SEM) and small angle X-ray scattering (SAXS).

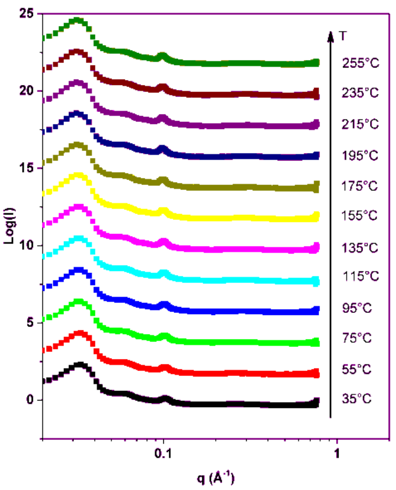

Fig.1: 1D SAXS profiles of PLMA-*b*-PMAA DBC with f_{PLMA} = 0.5 at different temperatures.

In the present study, morphological deviations compared with that of the conventional DBC phase diagrams in agreement with the theoretical studies is experimentally proved. Also, conductivities of the current DBC system at different lithium salt concentrations were measured and discussed in relation to the evolved morphologies.

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Grey Energy of Construction Materials

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With increasing building efficiency during their operation phase, the energy spent for construction and demolition of a building becomes more and more relevant if the entire life cycle of a building is considered. Therefore, the focus of research into energy consumption of buildings shifts to the construction and end of life phases and hence the embedded energy. For the related calculations background data from different databases is used. The study first clarifies the terms “grey energy” and cumulative energy demand, which are not unequivocally defined throughout Europe. In an extensive database comparison, embedded energy values for construction materials are collected and juxtaposed to identify differences and concurrences. It concludes that large differences can be shown, such that under certain conditions even the ranking of the materials can differ from database to database.

A definition of “grey energy” of a construction material can be found in the Swiss memorandum SIA 2032, which defines it to be “the total amount of non-renewable primary energy necessary for all processes, from the exploitation of raw materials through manufacturing and processing up to disposal”. In other words, it is the total non-renewable cumulative energy demand. In Germany, instead of a definition of “grey energy”, there exists a memorandum (VDI 4600) defining the Cumulative Energy Demand, comprised of renewable and non-renewable energy for manufacturing, use and disposal of a product or a service. Therefore, the study compares both non-renewable and renewable embedded energy divided into the energy demand for manufacturing and end of life of a construction material.

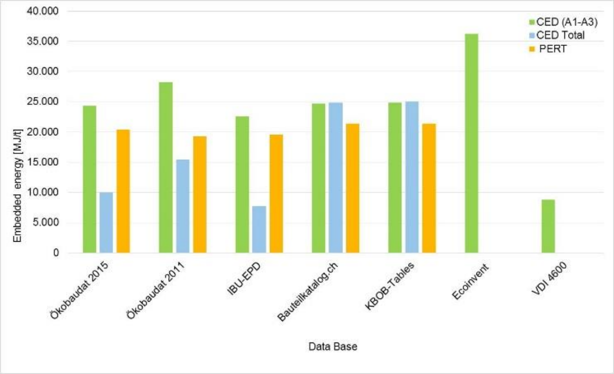

Figure 1: Embedded energy data for wood

Fig. 1 visualizes the comparison for construction grade lumber, the dataset with the largest differences. It shows data gaps and an order of magnitude of the results differing by a factor of about 4. In this particular case, this can be identified as a problem of outdated data, since the data in VDI 4600 is from a study conducted in 1999. Furthermore, it is possible that the renewable energy that is consumed in the growth process of wood has been neglected.

The ranking of the building materials within the database also varies. Per 1t of weight, concrete contains the smallest amount of total primary energy (PER) in all databases, aluminum the most. However, mineral wool and lumber are rated very differently depending on the database (fig. 2).

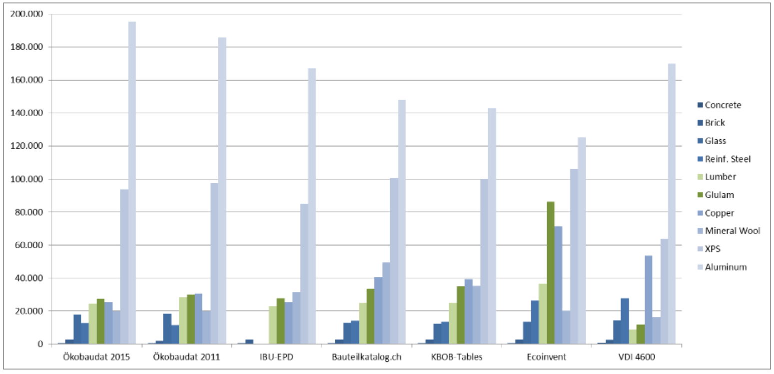

Figure 2: dataset comparison for all materials: total primary energy demand (cradle to gate)

The calculation of “grey energy” data is an important part of a holistic approach to sustainable building. The study concludes that further research and standardization is necessary to harmonize the data, make them more transparent and thereby arrive at an unequivocal approach to the evaluation of embedded energy.

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Foam-like structure of spray coated titania films for perovskite solar cells

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Due to a high surface-to-volume ratio and the bicontinuous morphology, foam-like nanostructures are receiving a growing interest in photovoltaics. Controlling the pore size is crucial for the photovoltaic applications, such as dye-sensitized solar cells (DSSCs) and hybrid solid state solar cells. In this study, spray coating is used, which is deposition method enabling up-scaling. In general, spray coating allows for a layer-by-layer deposition, which involves a highly dynamic size distribution of droplets atomized by a carrier gas. In this method, the spray solution can be organic solutions, polymers with poor solubility, as well as hybrid materials, such as colloidal nanoparticles and wet powder suspensions.

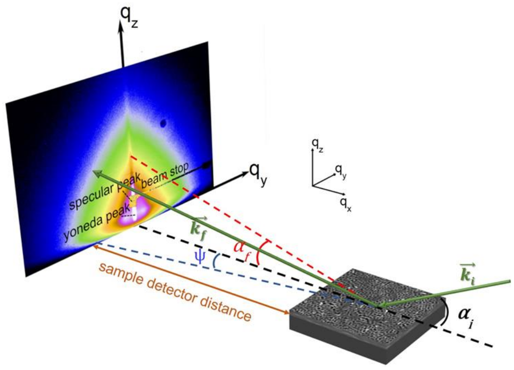

Figure 1. Schematic view of the GISAXS geometry: The incident angle of the incoming X-ray beam (k_i) is α_i and the exit angle of the scattered X-ray beam (k_f) is α_f. A beam stop is placed on the specular beam position.

To fully understand the mechanisms in the spray process, *in situ* grazing incidence small angle X-ray scattering (*in situ* GISAXS) is applied in the present study. GISAXS is an advanced scattering technique to probe the inner structures on the nanometer scale, which complements the observation of the surface morphology obtained from real space imaging techniques, such as optical microscopy, scanning electron microscope and atomic force microscopy. It can combine information about all relevant length scales in photovoltaics and inner film morphologies, which mainly effect the charge carrier generation in photovoltaic applications. Investigating the *in situ* dynamic and fast spray process is a big challenge for the real-space imaging techniques, due to lack of high temporal resolution. To overcome the difficulty, the spray set up is built up with for in situ GISAXS at the beamline P03 at PETRA III, DESY (Hamburg, Germany).

By using a two-step spin-coating procedure, the MAPbI$_3$ films is deposited on spray coated films, followed by spiro-OMeTAD as a hole transfer layer and gold layer as a counter electrode. The solar cell was characterized by J-V measurement, IPCE and SEM.

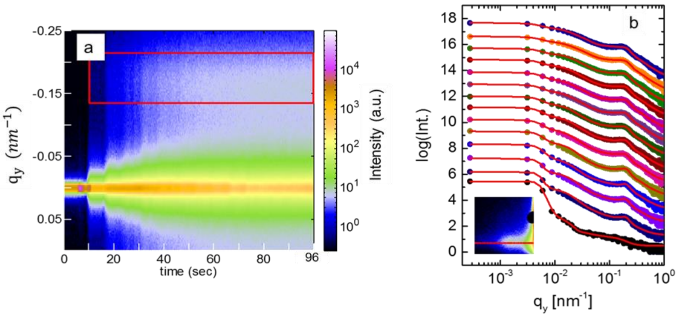

Figure 2. a) Full real-time mapping of horizontal cuts collected from in situ GISAXS data at $q_z = 0.35\ \mathrm{nm}^{-1}$. b) Selected logarithmic plots of integrated horizontal cuts (solid dots), and fits (red solid lines). All the curves are shifted along the y-axis for clarity. The plots from bottom to top present the in situ time in a varied range from 2 s, 12 s, 18 s, 24 s, 30 s, 36 s, 42 s, 48 s, 54 s, 60 s, 66 s, 72 s, 78 s, and 96 s, respectively.

Crystallization behavior of hybrid perovskite films on mesoporous titania templates

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In order to overcome the commercially available silicon solar cells which are known to be heavy, immobile and expensive, the research in thin film photovoltaics attracts high interest. Amongst these thin film techniques the organometal trihalide perovskite solar cells gained a tremendous efficiency improvement over the last years and exhibit tunable optical properties, which makes them favorable for a broad bunch of electronical and optical applications.
These perovskites are classified by the general formula ABX_3, where A indicates an organic cation (Methylammonium (MA) or formamidinium (FA)), B is an inorganic cation (Sn, Pb) and X are halides (Cl, Br, I), which act as anions. By varying the ratio of the halide atoms or involving some organic additives, like octylamine [1], the optical bandgap of the perovskite can be tuned continuously over a wide range. However, perovskites are known to degrade in moist environment [2]. Comparing the stability of methylammonium lead halide materials, methylammonium lead bromide ($MAPbBr_3$) is a promising candidate.
The perovskites can be crystallized by different techniques like spin-coating, dip-coating or vapor deposition and also no ultra-high vacuum is needed in the fabrication step [3].

The used fabrication procedure is shown in Figure 1. After deposing a TiO_2 hole blocking layer on the conducting FTO glass ((a), (b) and (c)) we spin-coat mesoporous titania which acts as an electron transport material. This layer enhances the final device performance with respect to the hysteresis in the current-voltage characteristics, which is often observed in perovskite solar cells. The perovskite is spin-coated via an one-step process on the titania template and annealed ((g) and (h)). On top we deposit the hole-transport material (HTM) spiro-OMeTAD and the gold counter electrode. We probed the morphology and crystallinity of the perovskite film, which exhibits quantum confinement [1] due to the used additive, on mesoporous titania via scanning electron microscopy (SEM) and X-Ray Diffraction (XRD). We also characterize the electrical and optical properties of the films and report the impact of the crystallinity of the perovskite film on the mesoporous titania in the final perovskite solar cell performance.

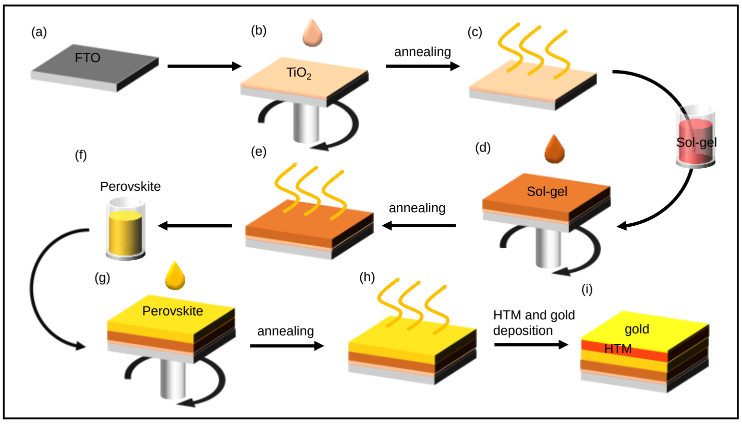

Figure 1: Fabrication process of the perovskite solar cell

References:
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Smart Grid: Cellular Communication Perspective

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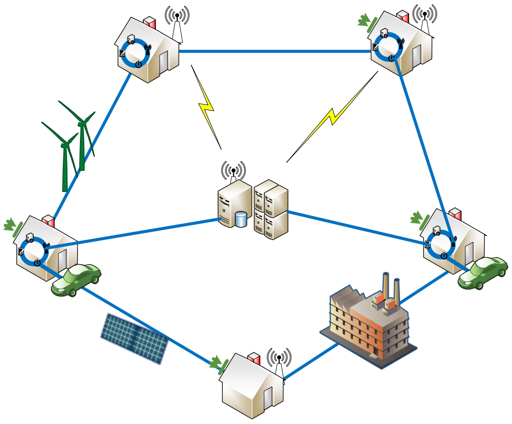
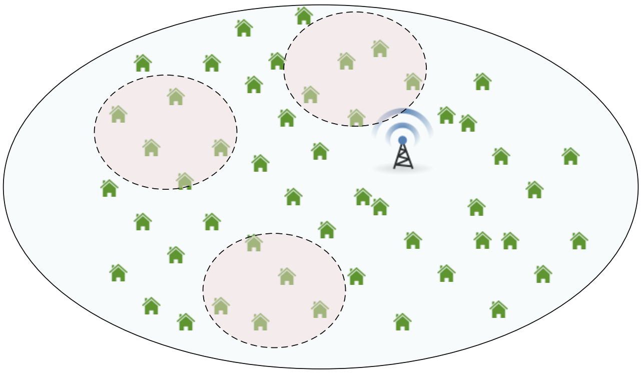
One of the enabling factors for creating novel power grids – also known as smart grids – are tools and approaches for making use of the large amount of data generated by the future grids. It can be data about the production or consumption, demands and available resources, or monitoring data of operational power systems. However, in order to do the processing, the data has to be first gathered, and then delivered to the place where it can be used.



Since a typical power grid spans a large geographical area, the communication infrastructure plays a key role in the data delivery, and can potentially become a bottleneck. The delivery might be delayed, hence, making the data outdated, or it can be fully lost due to insufficient communication resources.

In this presentation, we focus on the cellular networks, such as LTE-Advanced and upcoming 5G and their application in a smart grid scenario. We discuss main properties and peculiarities of power systems as communication agents, and outline the respective challenges for the communication.

In the second part of the presentation, we focus on a specific bottleneck of the existing cellular systems, namely on the overload during the connection establishment – random access (RA) – procedure. We explain the implications of RA on the power systems, discuss the state-of-the-art means for avoiding the overload during RA.



Finally, our approach to solve the random access problem is presented: throughput-maximizing resource allocation and clustered uplink aggregation. In throughput-maximizing allocation, the novel resource allocation scheme is presented, which allows prioritization of difference classes of accessing devices. For clustered RA, we discuss different option for aggregating the data packets generated by different users, in order to reduce the signalling overhead, and, thus, mitigate the network overload. We further present the analysis of different trade-offs associated with clustered data aggregation, and illustrate its performance analytically and simulatively.

Anodic oxidation of carbon and electrolyte with different conducting salts in high-voltage lithium-ion batteries

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Recently, many research activities have been devoted to the development of near 5 V cathode materials, e.g. $LiMn_{1.5}Ni_{0.5}O_4$ spinel, in order to raise the energy density of lithium-ion batteries and to allow for longer driving ranges of battery electric vehicles.[1] However, the enhanced degradation of carbon and electrolyte by the use of these high-voltage cathodes could not be mitigated so far. It was demonstrated by On-line Electrochemical Mass-Spectrometry[2] recently, that the anodic oxidation of conductive carbon, carbon coatings, and electrolyte at ≈5.0 V can be substantial at high temperature and in the presence of trace water, posing significant challenges for the implementation of 5 V cathode materials.[3,4] While these studies were done with $LiClO_4$ as conducting salt in order to study the effect of H_2O addition on oxidation without side reactions of salt and water, e.g. HF formation, we want investigate now to which extent the lithium salt can influence gas generation at high voltage. OEMS is used in combination with our newly developed two-compartment cell[3] to compare three types of lithium salts in terms of their influence on the anodic stability (close to 5 V) of electrolyte and conductive carbon in the battery cell. These are the commercially used salt $LiPF_6$, the sulfur and nitrogen containing LiTFSI, and the fluorine-free and oxygen containing compound $LiClO_4$. The salts are mixed with ethylene carbonate (EC) at a concentration of 1.5 M, so that linear carbonates like EMC or DMC which have a much higher vapor pressure than EC can be avoided, allowing for precise signal quantification in OEMS.[3] The comparison of the salts will be done on the basis of the CO/CO_2 gas evolution monitored by OEMS at various temperatures between 25 and 60°C. We employ a fully ^{13}C-labeled carbon electrode to deconvolute the CO/CO_2 evolution from electrolyte oxidation (^{12}C) from that of the conductive carbon oxidation (^{13}C)(see Figure 1). By quantification of both CO/CO_2 isotopes we determine the molar oxidation rate and the weight loss of electrolyte and carbon due to anodic oxidation. In summary, this study elucidates to which extent the lithium salt can influence gas generation at high voltage and might allow to deduce design principles for the synthesis of novel electrolyte salts.

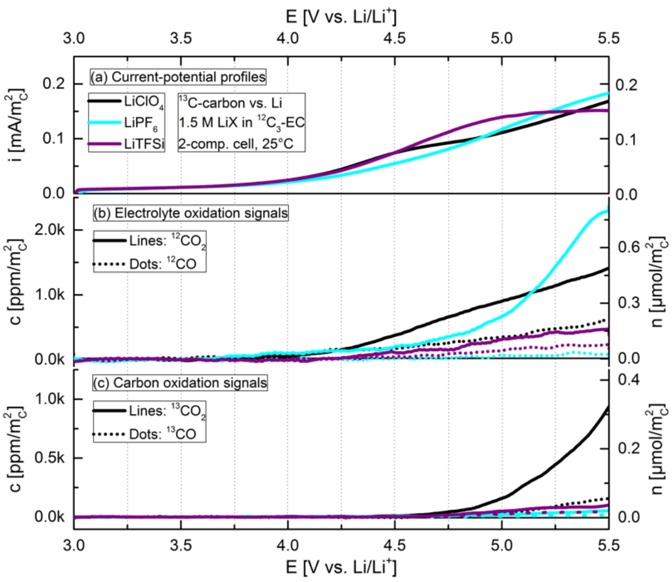

Figure 1: Carbon and electrolyte oxidation upon linear potential sweep from OCV to 5.5 V vs. Li/Li$^+$ at 0.1 mV/s with a ^{13}C-carbon working-electrode and a metallic lithium counter-electrode for an EC-based electrolyte with 1.5 M $LiClO_4$, $LiPF_6$, or LiTFSI respectively. (a): current-potential profile, (b): $^{12}CO/^{12}CO_2$ from electrolyte oxidation, (b): $^{13}CO/^{13}CO_2$ from carbon oxidation.

Acknowledgement

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Nanostructured zinc oxide films for application in hybrid photovoltaics

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Hybrid solar cells, a combination of conventional inorganic and organic photovoltaic systems, offer outstanding potential due to their minor investment compared to inorganic solar cells and higher stability compared to organic solar cells. In this kind of cells, nanostructured inorganic metal oxides with tunable morphologies are of great importance. Among the inorganic metal oxides, ZnO has been widely explored due to its outstanding electrical and optical properties and rich variety of morphologies. To date, many different routes towards ZnO nanostructures have been reported, such as hydrothermal synthesis, metal–organic chemical vapor deposition and so on, of which sol-gel process is one of the most widely used methods in solar cells due to the production of a homogeneous material and fabrication of ceramic coatings from solutions by chemical means. However, the structures obtained by the sol-gel process are limited, regarding both morphologies and structure sizes. A possible way to improve the film structure is to introduce amphiphilic block copolymers into sol-gel process. The hydrophilic and hydrophobic polymer blocks of amphiphilic block copolymers are covalently bound, which could modify the interface of ZnO.

GISAXS is a powerful analysis tool, which could detect the nanostructure inside thin films. In order to determine the structure formation process, in situ spray-deposited composite films were measured. Moreover, SEM and TEM were detected to investigate the surface morphology of the composite. The optical properties are examined with UV/Vis spectroscopy and the thickness is investigated by profilometry measurements. Aim is to increase the power conversion efficiencies of the solar cells.

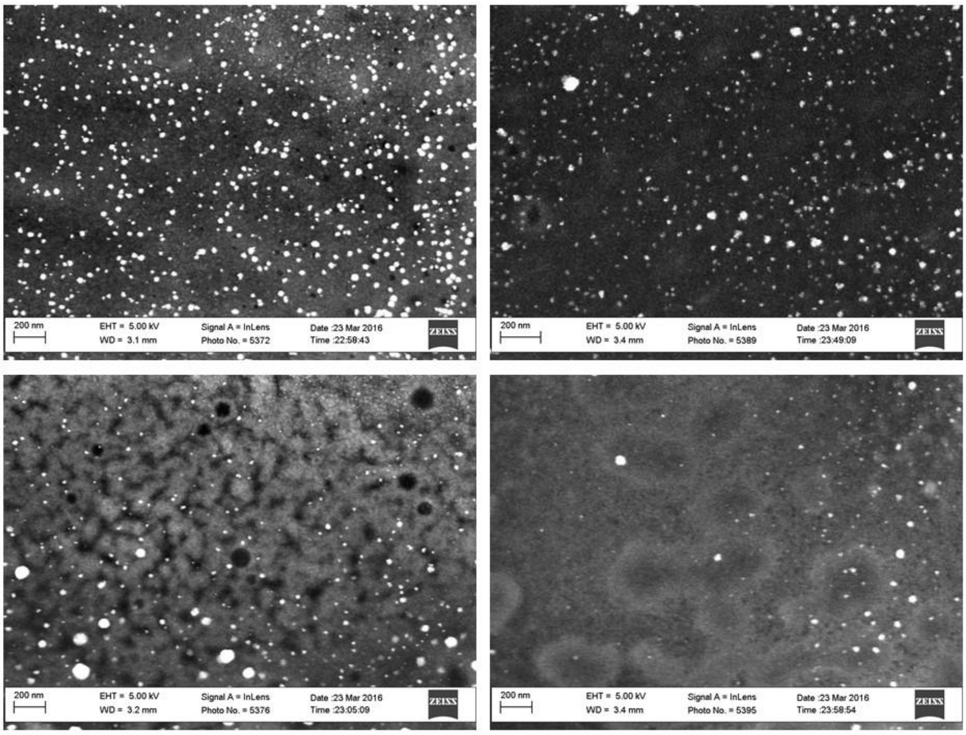

Fig.1: SEM images of the prepared composites

Morphology and Optoelectronic Properties of P3HT-b-PS/PCBM bulk heterojunction system in organic photovoltaic application

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In order to implement organic photovoltaic (OPV) into daily life application, researchers have performed dedicated studies to improve the device efficiency and stability. An optimum functional OPV device requires an interpenetrating bulk heterojunction (BHJ) network, in which the nanoscale morphology is constrained in the same scale of exciton diffusion length (~10nm). The resulting film morphology is thereby crucial to guarantee the device performance. As diblock copolymer possesses the property to microphase separate into well-defined nanostructure, this kind of materials is of particular interest to be applied as active layers for OPV applications.

In the present work, we blend the conjugated diblock copolymer P3HT-b-PS with the fullerene derivative PCBM. The local surface morphology is determined by atomic force microscopy (AFM) and the average film morphology by neutron scattering. Due to the PCBM molecule fast diffusion into the amorphous P3HT regions, the neutron scattering contrast is enhanced between the two blocks of copolymer. The information about nanoscale lateral structures is achieved by applying grazing incidence small angle neutron scattering (GISANS). In addition, x-ray reflectivity (XRR) reveals the vertical composition. Optoelectronic properties are determined by absorption and photoluminescence measurements.

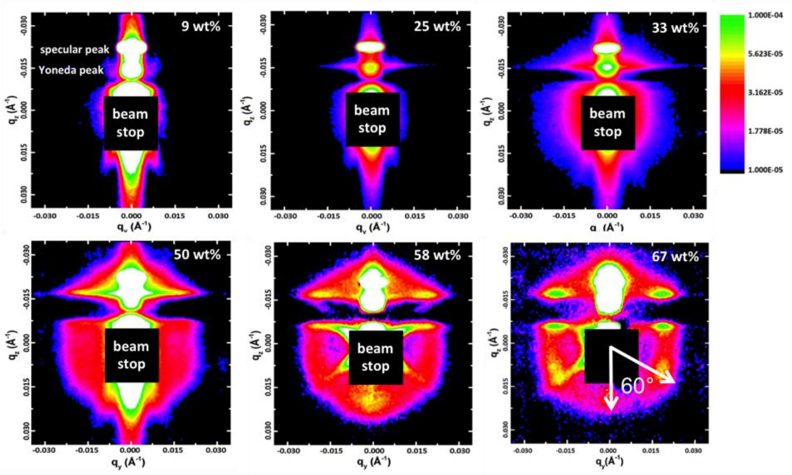

Figure 1. 2D GISANS patterns of P3HT-b-PS/PCBM bulk heterojunction system with 6 different PCBM weight fractions. Hexagonal orientation appears at a PCBM weight fraction of 67%.

Molecular Beam Epitaxy and Characterization of InGaN Nanowires on Si (111)

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Multi-junction solar cells have received wide attention as each cell can absorb different wavelengths of the solar spectrum which leads to an increased energy conversion efficiency.

InGaN has a variable band gap from 0.7 to 3.4eV that covers nearly the whole solar spectrum. Combined with Si, theoretical considerations show that an InGaN/Si tandem solar cell could be an optimal implementation of a double-junction cell [1]. Especially at an In content of 46%, it is expected that a resonant tunnel junction is formed between both cells (Figure 1).

Furthermore, the cell efficiency could be increased by growing nanowires to enhance optical properties such as efficient light trapping and to reduce structural defects due to lattice and thermal mismatch acting as unwanted recombination centers (Figure 2).

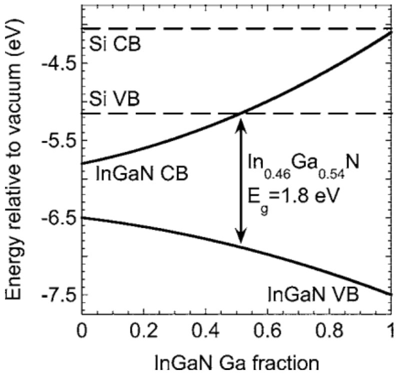

Fig. 1: Energy diagram showing the conduction and valence bands of InGaN as a function of alloy composition in comparison to the conduction and valence bands of Si

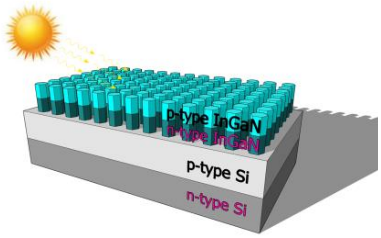

Fig. 2: Sketch of an InGaN nanowire/Si tandem solar cell.

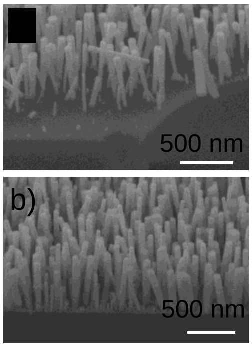

Fig. 3: Tilted-view SEM image of a) InN nanowires and of b) InGaN nanowires on Si (111).

As first step towards such an InGaN/Si solar cell, the growth of high quality InN nanowires directly on Si(111) substrates by molecular beam epitaxy has been studied. By varying the relevant growth parameters, namely substrate temperature and III/V-ratio, different growth regimes were identified and the InN nanowire growth was optimized (Figure 3a).

As a next step the growth of InGaN nanowires with different Ga content was investigated (Figure 3b). Recent results on the structural and optoelectronic properties of InGaN nanowires on Si obtained by energy dispersive X-ray spectroscopy, Raman spectroscopy and conductive AFM measurements will be presented.

High temperature fuel cell in micro combined heat and power generation

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The combined generation of heat and power is a very efficient decentralized technology to simultaneously supply buildings with electricity and heat. Recently, besides conventional micro combined heat and power (mCHP) units, small high temperature fuel cells have appeared on the market. This research focuses on such a system, which has a constant electrical output of 1.5 kW and a varying thermal output of up to 0.85 kW. The electrical efficiency is around 60 %, so comparable to state of the art centralized combined cycle power plants. Furthermore, the waste heat can be used to provide hot water for buildings and increase the overall efficiency up to 85 %. Since fuel cells generate heat and power with cold combustion of gas, the thermal output characteristics are different to conventional mCHP units. Accordingly, the conventional heating system must be adapted to achieve the high overall efficiency.

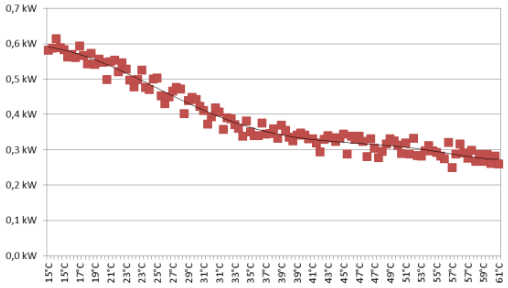

Figure 1: Thermal power output depends on return temperature (RT)

Before the heating system can be adapted, the specific characteristics of the fuel cell have to be measured. As shown in figure 1 the thermal power is cut to half over the given return temperature (RT), different to conventional mCHP units. So it is essential to maintain a low RT in favor to reach a high overall efficiency. After measuring the characteristics, these are modeled with a dynamic energy simulation tool (see figure 2). With this tool a single family home (SFH) is simulated over one year with a conventional hot water system and an underfloor heating system. The results show that only 35 % of the waste heat can be used, which are an equivalent of a heat power output of only 0.3 kW [1]. To optimize the heat output it is crucial to minimize the RT to the fuel cell. Usually the fuel cell is directly connected to a hot water storage, so the management of the storage temperature defines the RT. Hence the primary goal is to decrease the heat storage temperature to a minimum. Usually the storage temperature is around 60°C to avoid legionella. With some system adjustment the temperature can be reduced to 45°C, since this is the minimum hot water tap temperature. Furthermore, the temperature is reduced to 35°C, which is only sufficient for heating purposes. For drinking hot water, it is heated to 45°C with a flow-through electrical heater. With these two measures the thermal output and the efficiency can be increased. The temperature reduction to 45°C increases the thermal power to nearly 50 %. The further reduction leads to 56 % usage of the waste heat. But only the reduction of the storage temperature to 45°C has an economic sense, because the additional cost of the needed electrical heater for a 35°C storage temperature does not payback. Nevertheless, the primary energy demand of the building is reduced with the two measures to zero [1].

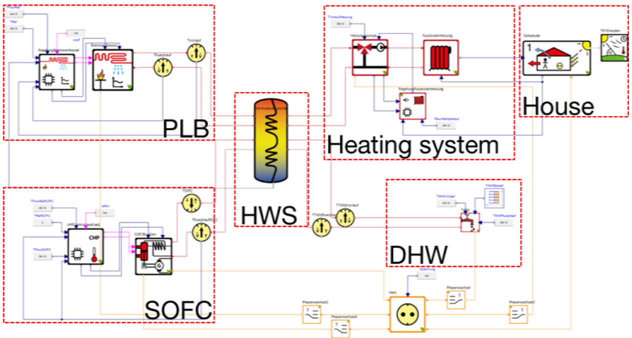

Figure 2: Model in SimulationX

Besides showing the possibilities to improve the heat output, the simulation also made clear that an additional heater is need. Usually a gas condensing boiler is combined with the fuel cell. Research showed that a small heat pump is more favorable concerning costs and primary energy [2]. Furthermore, a fuel cell paired with a heat pump can be an interesting player in the future energy market. The system can deliver positive and negative loads in connection of virtual power plants.

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The influence of light intensity on the performance of organic solar cells

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In recent years the contribution of renewable energy to the energy market has grown significantly. An important sector of renewable energy is using photovoltaics (PV) technology. Currently, most solar cells installed on roof tops are based on silicon technology. The market shares of PV in the EU increased from 2000 to 2014 from 0 to 9,7 % [1]. However, one disadvantage of the silicon solar cell technology is the high cost of production due to the intrinsically energy consuming production process. An attractive alternative are organic solar cells (OSC) currently still in the research phase. OSCs are solution processable and can therefore be printed which promises very low production costs. Furthermore, this production method is well established in other technologies and offers the possibility for large scale processing. Additionally, OSCs have light weight and are flexible which allows exciting and new areas for application which are not feasible with current technology.

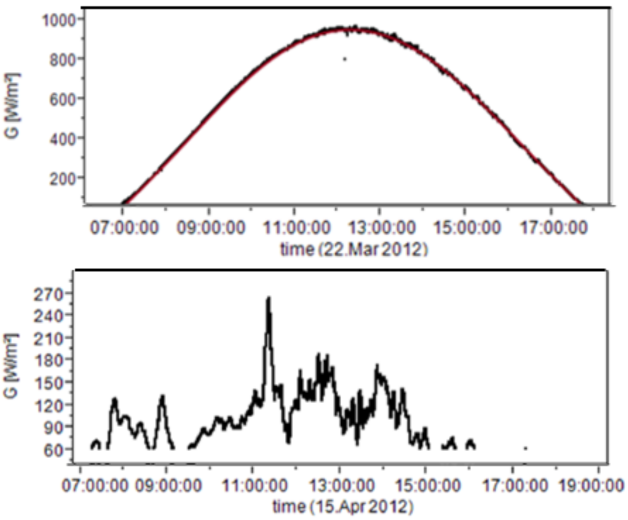

Figure 1: Solar irradiance in W/m^2 on a 22.03.2012, a sunny day (top) and on 15.04.2012, an overcast, cloudy day (bottom). Data is taken in Garching, Germany.

For solar cells to convert a maximum of solar energy to electricity a technology needs to be chosen that can effectively convert solar energy at various light intensities and temperatures. As shown in Figure 1, the light incident on any PV installation varies strongly with the weather. The data shown is recorded in Garching, Germany [3] on a sunny (top) and cloudy day (bottom). If the sky is clear almost 1000W/m^2 are incident at noon, which corresponds to standardized testing conditions for PV modules. However, as can be seen in the Figure 1, at many more times this value is not achieved. We are therefore interested in the performance of organic solar cells in varying light conditions and temperatures. To characterize different material systems, it is necessary to measure the IV curves of the solar cells at different light intensities.

To systematically study the light intensity – efficiency relationship we are extending the standard sun simulator to an automated setup which will measure the organic solar cells at varying light intensity.

References:

[1] European Wind Energy Association, 2014 European Statistics, status Feburary 2015
[3] Diploma Thesis, Yvonne Boose, TUM, 2012

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Implementation of buildings with fluid-flown glass façade on district level

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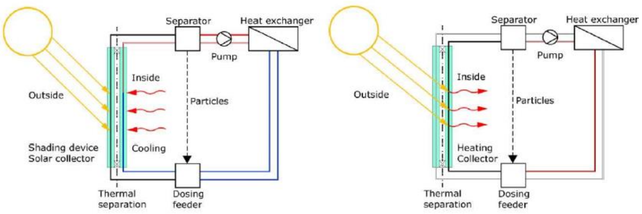

Figure 1: Basic operating modes of the fluid glass in summer (left) and winter (right) (Gstoehl D. et al. 2011)

In order to increase the building's energy efficiency and the usage of solar energy, a new and innovative concept of solar thermal glass façade is developed within the FLUIDGLASS project[1].

In the current approach the fluid glass façade consists of two layers, where the fluid is circulating in closed cycles. The fluid layers absorb the solar radiation and functions as solar thermal collector and overheating protection. The solar transmission through the fluid glass façade is controlled by coloring or decoloring the fluid layers. In cooling periods, the outer fluid layer will be dyed. Dyed fluids increases the absorption of solar radiation within the fluid and thus the collector efficiency of fluid glass. The solar heated fluid is circulated and used either within the building or externally. By tempering the inner fluid layer additionally, the fluid glass functions as a heating or cooling device. The inside and outside fluid layers are thermally separated. In Figure 1 two basic operating modes for summer and winter are illustrated.

In this work the potential of implementing buildings equipped with fluid glass façade through a low temperature network on district level is investigated. The concept of the network system is shown as follows: In summer, a high-rise office building with fluid glass façade is able to generate more thermal energy than its demand. The excess energy is charged into a seasonal heat storage within a low temperature network. In winter, the-high rise building and the residential buildings in the district connected to the network are supplied with the stored heat. Therefore, the excess heat from the fluid glass is used as a renewable heat source for the buildings. The inlet temperature from the network is lifted with heat pumps for the building's heating systems.

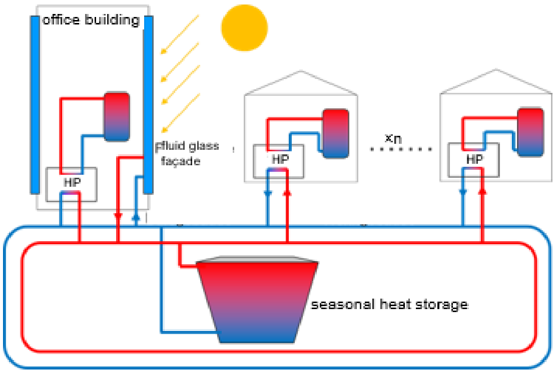

Figure 2: the scheme of the system

In order to prove the performance and potential benefits of the system, annual simulations at two different locations - Munich and Shanghai - were performed with the software ITI SimulationX. The important characteristic variables are calculated, e.g. the total electricity consumption, seasonal performance factor of the heat pump and chiller, temperature profile of the heat storage as well as solar heating. Finally, the effects to the systems' efficiency caused by the location and the dimensioning of heat storage are summarized and discussed.

As a conclusion it is proved that the system is generally suitable for a location with high heating demand and low cooling demand, e.g. Munich. Electrical energy demand up to approximately 27 % are investigated compared to a reference scenario with decentralized air-water heat pumps in every single building. Further investigations, e.g. with domestic hot water demand during heating period will be done within the FLUIDGLASS-project.

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Printing High Efficiency Solar Cells

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Due to the potential for generating electricity at a low cost and compatibility with flexible substrates required for roll-to-roll manufacturing, organic solar cells (OSCs) have attracted tremendous attention as an effective way to solve the energy crisis in the near future. At present, the power conversion efficiency (PCE) of OSCs devices has been demonstrated to be above 10%. However, translation to large-size-scale devices still keeping high PCE is a remaining challenge. Therefore, we focus on applying printing techniques to fabricate solar cells with high efficiencies.

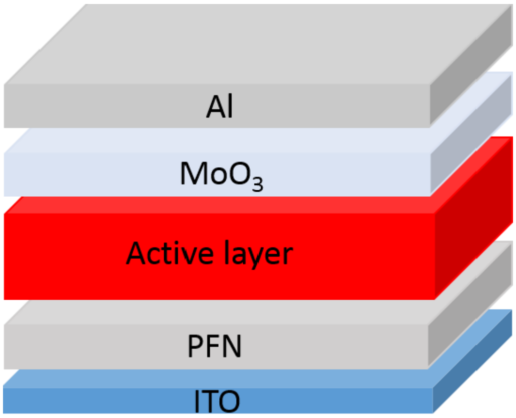
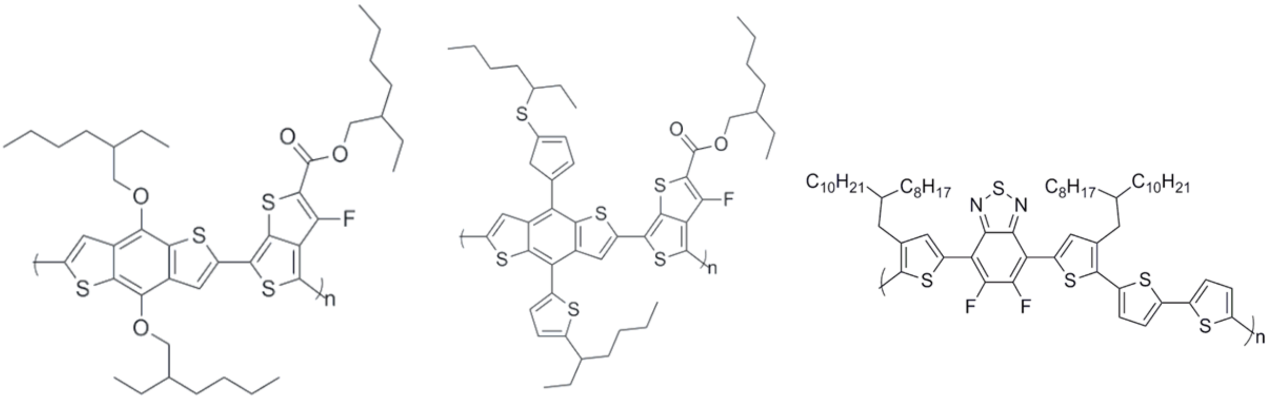


Figure 1. Schematic structure of the solar cell

In our work, the inverted device architecture is employed as this is known to be more stable. A thin layer of conjugated polymer, poly [(9, 9– bis (3'-(N, N-dimethylamino) propyl) -2, 7-fluorene)-alt-2, 7-(9, 9–dioctylfluorene)] (PFN), is applied as the hole blocking layer (see Fig. 1). The room temperature and solution processed PFN is favorable for flexible and large-scale roll-to-roll production. In the past few years, some new state-of-the-art low bandgap polymers with PCEs exceeding 9%, such as polythieno [3, 4-b]-thiophene-co-benzodithiophene (PTB7), poly[4,8-bis(5-(2-ethylhexyl)thiophen-2-yl) benzo[1,2-b;4,5-b'] di thiophene -2,6-diyl-alt- (4-(2-ethylhexyl)-3-fluorothieno[3,4-b] thiophene-) -2-carboxyl-ate -2-6-diyl)] (PTB7-Th) and poly[(5,6-difluoro-2,1,3-benzothiadi-azol-4,7-diyl)-alt-(3,3'''-di(2-octyl do decyl)- 2,2',5',2'',5'',2'''-quarter thiophen-5,5'''-diyl)] (PffBT4T-2OD) (see Fig. 2), have been developed as the most promising donor materials. So far, many investigations focus on these polymers just using spin-coating to make solar cells. In contrast, we intend to prepare solar cells by making use of printing techniques. The active layer will be deposited by printing instead of spin-coating. Afterwards, we measure the I-V curves under AM1.5 standard conditions to get the performance of photovoltaics devices. Moreover, advanced scattering techniques as for example grazing incidence small angle x-ray scattering (GISAXS) and grazing incidence wide angle x-ray scattering (GIWAXS) are applied to probe the morphology changes from spin coating to printing.



PTB7 PTB7-Th PffBT4T-2OD

Figure 2. Molecular structures of PTB7, PTB7-Th and PffBT4T-2OD

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