

Technische Universität München



# "Innovations for Energy Systems, Mobility, **Buildings and Materials**"

5th Colloquium of the Munich School of Engineering 09.07.2015

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The energy transition which was considered to be one of the outstanding projects of Germany policy lost pace in the recent time. Debates on nearly all issues have replaced the former consensus that a major change is necessary to establish a sustainable energy system on the long term. The controversies reached all questions starting from the best scheme to promote re-

newable energies over the possible installations of a new capacity market over discussions on new overhead lines and ends in all places where new wind turbines should be installed.

Science is more than ever asked to make clear that a new energy system is necessary and will create multiple benefits not only in Germany but worldwide when designed in a proper manner. Science is also asked to help in all the multiple debates to bring sound arguments which help to decide which options should be pushed forward.

At the end of the year world governments will gather in Paris to discuss a treaty to curb cabon dioxide emissions worldwide. Only with new and advanced technology this goal can be reached.

The Munich School of Engineering is making its contribution by catalyzing new projects in the university and by participation in the outside debate if required. In our annual meeting our young researchers will present their work together with key note speakers coming from eminent research centers.

The MSE is looking forward to your participation.

Thomas Hamacher Director Munich School of Engineering

### **Munich School of Engineering (MSE)**

The **Munich School of Engineering (MSE)** of the Technische Universität München is based on an innovative concept motivated by the demand for the de-compartmentalization of the conventional engineering disciplines: the combination of interdisciplinary research and cross-faculty teaching. The MSE is institutionalized as an Integrative Research Center with doctorate-granting rights.

**TUM.Energy** is a cross-faculty research initiative within the Munich School of Engineering which offers a platform for the "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 faculties 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 **Study Program Division** of the Munich School of Engineering (MSE) provides currently three degree courses with the 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, results of fundamental research in engineering and science as well as entrepreneurial viability of new technologies. This combination opens the MSE-graduates great professional opportunities in the interdisciplinary business fields of the future.

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 course allows students to individually create their personalized specialization within engineering. The course *Industrial Biotechnology* (Master of Science) qualifies graduates of science or engineering bachelor study programs in the field of white biotechnology. Therefore, the four semester curriculum contains subjects of a wide spectrum regarding life and food science as well as process engineering, chemistry, physics, agronomy, robotics and information technology.

The MSc *Human Factors Engineering* enables graduates to design the information flow and new forms of interaction concepts between users and technical systems. They can enhance the anthropometric design of workplaces from industrial production to aviation cockpits. Students learn the skills needed to succeed in academic or industrial research, production, safety management, or counselling.

The orientation program *studium MINT*, launched in summer semester 2014, provides High School Graduates interested in MINT (STEM) disciplines with a solid information and knowledge fundament for their study and career choice. It allows them to get in touch with different scientific disciplines and thus find out where their individual interests and strengths lie before enrolling in a certain study program.

### **Center for Power Generation**

The Center for Power Generation (CPG) is a research cooperation established within the MSE and involving multiple TUM institutes which deal with research on energy conversion. Apart from efficient and innovative power plant technologies, the research spectrum also includes innovative research on transportation and storage of electricity, control system, and new, optimized technologies to reduce greenhouse gas emissions. 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.

The research project "Energy Valley Bavaria - Flexible Power Plants" is an example for CPG's interdisciplinary research. Experimental investigations of combustion and evaporation are combined with theoretical approaches of power plant simulation and power system optimization. Furthermore, new innovative projects have been developed regarding geothermal power plant technology, energy storage with power-tofuel, or innovative energy solution at the Campus Garching ("CleanTechCampus").

To date 17 partners from 4 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 "SolarTechnologies 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 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 Climatology and Building Services, Energy Efficient and Sustainable Design and Building as well as Energy Economics and Application Technology, 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 CO2 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.

### Programme

### 8.30 - 9.00 am

Registration

#### 9.00 - 9.15 am

**Opening** Klaus Diepold, Senior Vice President TUM Thomas Hamacher, Director Munich School of Engineering

#### 9.15 - 9.45 am

Keynote: The Energiewende as a Business Case Clemens Hoffmann, Director Fraunhofer Institute for Wind Energy and Energy System Technology (IWES)

#### 9.45 - 11 .00 am

Session Chair: Markus Lienkamp, WZE MSE

#### Energy Storage System Management and Design Space Exploration of Public Electric Vehicle Charging Stations

Sangyoung Park, Institute for Real-Time Computer Systems

From Model Surfaces to Nanostructured Catalysts for Oxygen Electroreduction in Fuel Cells Viktor Colic, Physics of Energy Conversion and Storage

Visio.M - Light Vehicle Concept for Urban Electric Mobility

Patrick Stenner, Institute of Automotive Technology

11.00 - 11.45 am Poster Presentation, Coffee Break

11.45 - 1.00 pm Session Chair: Werner Lang, ZNB MSE

Design-Engineering-Based and Material-Based Improvement of Precast Concrete Facade Elements Matthias Pätzold, Chair of Building Construction and Material Science

Non-Residential Buildings - Modelling the Long-Term Development of Energy Demand Laura Franke, Center for Sustainable Building

The CityGML Energy ADE - An International Standardization Effort for the Extension of 3D City Models to Support Energetic Building Analysis Robert Kaden, Chair of Geoinformatics

1.00 - 2.30 pm Poster Presentation, Lunch Break

#### 2.30 - 2.50 pm

Teaching at MSE Nikolaus A. Adams, Dean for Academic Affairs MSE

#### 2.50 - 4.05 pm

Session Chair: Peter Müller-Buschbaum, NRG MSE

Optimization of Carbon Nanotubes Networks for Organic Photovoltaics by Femtosecond Laser Structuring

Jürgen Sotrop, Institute for Nanoelectronics in cooperation with University of Applied Sciences Munich

Metal Cluster Semiconductor Hybrid Materials in Photocatalysis for Chemical Energy Conversion Constantin Walenta, Chair of Physical Chemistry

Hybrid Thermoelectrics Based on a Polymer-Nanoparticle Composite Nitin Saxena, Chair of Functional Materials

4.05 - 4.50 pm Poster Presentation, Coffee Break

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

Heat Transfer at Supercritical Pressures in Power Applications - Physics and Experimental Methods Gerrit Schatte, Institute for Energy Systems

#### Optimal Planning of Urban Infrastructure Networks for Multiple Energy Carriers Johannes Dorfner, Institute for Renewable and Sustain-

able Energy Systems

Small-Scale Wind Turbine Systems with Efficient and Inexpensive Generator Topology for Micro-Grids Christoph Hackl, Research Group MSE

#### 6.05 - 6.35 pm

**Keynote: Building and Energy Research in Singapore** Priya Pawar, Energy Research Institute, Nanyang Technological University, Singapore

6.35 - 6.50 pm Summary of the Day

6.50 - 9.00 pm Poster and Presentation Award, Colloquium Dinner 1 Oral presentations



### **Energy Storage System Management and Design** Space Exploration of Public Electric Vehicle Charging **Stations**

Sangyoung Park<sup>a</sup>, Alma Pröbstl<sup>b</sup>, Wan Li Chang<sup>c</sup>, Abhisek Ukil<sup>d</sup>, and Samarjit Chakraborty<sup>e</sup>

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Fig. 1: EV charging station architecture

Lack of electric vehicle (EV) charging infrastructure is one of the major limiting factors for wide adoption of EVs. EVs suffer from long charging time and short-drive range limiting EV usage to daily short-range commuting rather than general purpose long-range travels. While numerous EV charging infrastructures have been proposed, public charging station architecture is crucial to support long-range travel of EVs which require multiple charging cycles. This work focuses on public EV charging station architecture comprising PV panels, an energy storage system (ESS) and multiple fast-DC charging posts and propose an ESS management algorithm for operating income optimization. We justify the use of each comprising element from an

economical perspective by exploring the design space under objective of maximizing return on investment. The operating income maximization problem is formulated as an average reward Markov decision process (MDP) maximization problem and solved using value iteration method. We also perform design space exploration of ESS and PV panel sizing for a number of scenarios on future ESS cost, PV panel cost and grid electricity price. The proposed solution method exhibits up to 28% improvement in amortized cost compared with no PV, no ESS case under optimistic scenarios.

Formulation of the optimization problem involves stochastic modeling of the solar irradiance and EV charging traffic patterns. Together with the stochastic models, detailed models of the comprising components, that is PV panel, ESS, are combined to build a transition probability matrix (TPM) transition reward matrix (TRM), which eventually synthesizes a controller that determines state of charge (SOC) level for the charging station ESS using relative iteration algorithm. Example case of power flow in the EV charging station for four days is shown in Figure 2. Use of PV panels and an ESS is indeed beneficial in terms of operating cost reduction as can be seen from Figure 3. However, as high installation costs of PV panels and ESS harms profitability and thus depreciation analysis should be performed accordingly. The amortized cost considering depreciation of PV panels and ESS for various combinations of sizes of PV panel and ESS is shown in Figure 4. Under current ESS costs, which is closer to 500 USD/kWh, an ESS is hardly beneficial (always higher cost than baseline). However, under futuristic scenarios of cost projection, there is up to 28% anticipated cost saving from utilizing ESS and PV panels.



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## From model surfaces to nanostructured catalysts for oxygen electroreduction in fuel cells

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Polymer electrolyte membrane fuel cells (PEMFCs) are a promising alternative for traditional energy sources, especially internal combustion engines. However, their more widespread application is hindered by the sluggish kinetics of the oxygen reduction reaction (ORR) taking place on the cathode. This results in a large overpotential required for ORR and high platinum loadings necessary to catalyze the reaction, greatly increasing the operational costs. Hence, finding more efficient and stable new catalysts for the ORR is of paramount significance for the wider implementation of PEMFCs.

It is now well understood that an ideal catalyst for the ORR should bind the reaction intermediates approximately 0.1eV weaker compared to a model Pt(111) surface, and also be sufficiently stable under operational cell conditions. In order to increase the efficiency of real devices, alloys of Pt with late transition metals and lanthanides have been studied extensively, particularly in their nanoparticulate form. However, many of these alloys are far from being model surfaces and are not stable under the conditions in the PEMFC; the solute metal dissolves from the surface layers. In other words, the surface becomes dealloyed. This process results in a structure in which several Pt-enriched layers cover the bulk alloy and protect it from further dissolution. The system is difficult to model as the structure is complex and highly dependent on preparation methods.

In this work, we propose a simple method to predict the activity of dealloyed PtnX alloys towards ORR. Specifically, given that the Pt overlayer is several atomic layers thick, we suggest that the strain effects dominate and are primarily determining the behavior of these alloys. The strain in the system is the result of the differences between the lattice parameters of the alloy on one hand, and Pt on the other, which, depending on the nature of the solute metal, results in different compressive strains in the lattice of the platinum overlayer after dealloying. This causes changes in the electronic structure, and, consequently, the binding properties of the electrode surface.

We propose that the atomic radius of the solute metal can be used as a simple descriptor to explain and predict the lattice strain, and consequently, the maximal catalytic activity of such alloys. The optimal amount of lattice strain will result in the weakening of the Pt-adsorbate bond for the ideal amount and, consequently, in the highest activity. Figure 1 shows two such maxima for atoms with radii being smaller or bigger than that of Pt. The implications of this phenomenon can be observed for instance in the activity trends of nanoparticulate alloys of Pt (Figure 2). While the ORR activity of the Pt-Y nanoparticles decreases with decreasing the particle size, the activity of Pt-Ni goes through a maximum. The approach we present explains this behavior by the fact that Ni introduces too much strain to the lattice so with the decrease of particle size the binding energy goes through the ideal value, which is not the case for Pt-Y (Fig 1).







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### Visio.M - Light vehicle concept for urban electric mobility

Patrick Stenner<sup>a</sup>, Prof. Dr.-Ing. Markus Lienkamp<sup>b</sup>

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Electric cars are silent and cause no emissions where they go. Therefore, they are considered an important option for future individual mobility in urban areas and beyond. But on the way to mass production of electric vehicles, there are still significant technological hurdles to overcome.

Within the joint research project Visio.M well-known companies of the German automotive industry, together with scientists from the Technische Universität München, explore how the price and safety of small, efficient electric vehicles can be brought to a level enabling them to achieve a significant share of the mass market.

The consortium partners explore innovations and new technologies for vehicle safety, propulsion, energy storage, and operational concepts for implementation under the framework requirements of large-scale production. Special attention is given to safety-related design issues. Despite minimal weight, Visio.M is expected to achieve a level of protection equal to that offered by conventional cars with combustion engines.

Participants in the Visio.M consortium are, in addition to the automotive companies BMW AG (lead manager) and Daimler AG, the Technische Universität München as a scientific partner, and Autoliv BV & Co. KG, the Federal Highway Research Institute (BAST), Continental Automotive GmbH, E.ON AG, Finepower GmbH, Hyve AG, IAV GmbH, InnoZ GmbH, Intermap Technologies GmbH, LION Smart GmbH, Neumayer Tekfor Holding GmbH, Siemens AG, Texas Instruments Germany GmbH and TÜV SÜD AG as industrial partners. The project is funded under the priority program "Key Technologies for Electric Mobility -STROM" of the Federal Ministry for Education and Research (BMBF).

www.visiom-automobile.de



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

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Fig. 1: Reinforcement of the outer layer



Fig. 2: x=number of storeys | y=wall- thickness



The research project examines the optimization of the external envelope of reinforced concrete structures with facing concrete external surfaces. The aim is to develop and evaluate new construction methods that reflect modern-day concerns such as the need for good insulation, the sustainable use of resources, the reduction of wall thicknesses and minimal consumption of resources, as well as the ability to quickly erect buildings in inner-city locations (with accordingly high land costs). The research project focuses in particular on optimizing insulation thickness and achieving good facing concrete surfaces.

Inner load bearing Layer: Prefabricated concrete walls allow us to produce high quality elements with an efficient use of thin concrete layers. Today, the production of concrete requires a lot of energy. Compared with timber, concrete and especially Semi Pressure Concrete has perfect fire prevention capabilities. The study focuses on increasing the use of regenerative energy. Inner walls made of 6cm thick UHPC or 8cm thick B50/60 SPC wall have proved to be suitable for buildings of up to 6 storeys. Fabrication is simpler for the latter method. The concrete matrix is reinforced by fiber-steel.

Middle insulation layer: Aerogel fleece pads of 0,013 W/mK can provide maximum insulation in a very thin layer. These pads do not have to be handled as carefully as VIPs. Fiberglass reinforcement carries the outer skin without thermal bridges.

Outer protecting layer: The 2-D and 3-D grid reinforced SPC facade elements can be fabricated in a highly automated process and, with the addition of milled recyclate, an attractive outer surfaces can be achieved.

Synopsis: The ability to produce the three-layered fiberreinforced composite cast panels in a highly automated factory process ensures a high performance structure. The sustainability will depend on the conservation of natural resources, and the analysis of the usage of recyclate and carbon-neutral admixtures. All in all, the new construction methods will enable the design of building structures with walls of maximum 25 centimetre thickness, highly effective insulation and attractive surfaces. In addition, the study also focuses on building physics and minimal construction time.

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## Non-Residential Buildings<sup>1</sup> – Modelling the Long-Term **Development of Energy Demand**

Laura Franke<sup>a</sup>, Isabell Nemeth<sup>b</sup>

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Figure 1: The role of non-residential buildings (NRB) compared to residential buildings (RB) in 2013/14 [1, 2, 3, 4], own presentation

### **RESEARCH APPROACH**

Latest statistics and estimates of the German building stock show that net floor space and energy demand of the non-residential building sector (NRB) play an important role in terms of building stock efficiency (Figure 1): although the share of NRBs is small (13%), they account for 27% of the total net floor space (~ 5 billion m<sup>2</sup>) and are responsible for more than one third of the building stock final

energy demand (~ 980 TWh) [1, 2, 3, 4]. Figure 1 indicates that on average NRBs have a 2.5 times larger net floor space per building than residential buildings (RBs), and a 1.5 times higher final energy demand per m<sup>2</sup> than RBs. Thus, the NRB energy efficiency potential deserves detailed investigation.

### **OBJECTIVES**

The overall aim of the research project is to utilize the currently underestimated energy saving potential of the NRB sector, enabling NRBs to contribute to meeting the latest German energy efficiency targets: a climate neutral building stock with 80 % reduction of the primary energy demand by 2050. To reach this goal, two aspects are of utmost importance: a deep understanding of building owner and investor decision-making, as well as a broad knowledge of the technical efficiency potential in the heterogeneous building sector (Figure 2). The investigation of the two aspects creates a basis for market-oriented action recommendations and



Figure 2: Façade examples of the heterogeneous NRB group [5], own presentation,

strategies, motivating investors and owners of NRBs to increase the energy efficiency of their buildings.

### **METHOD**

The research project started with the objective of investigating quantity structure and energy demand of the NRB sector and identifying the long-term energy saving potential of this group. From this initial aim, the following three subsequent research processes emerged: firstly, to create a reliable data base compensating for the current fundamental lack of NRB data; secondly, to develop a model that estimates the long-term energy demand of NRBs, and thirdly, to carry out a sensitivity analysis on parameters that influence the final energy demand. Hereby, crucial factors are: basic building parameters, life span of building components and technology, as well as ecological (climate change), social (demographic development), political (legal requirements), and economical (perspective of investors and owners) factors.

### PROSPECTS

The authors note the low significance of energy efficiency in the NRB sector, arguing for a more investorand owner-oriented system: using the proposed NRB model as a tool, individual and feasible energy saving concepts can be developed. This way, investors and owners identify themselves with the idea of benefitting from the investment in energy-oriented refurbishment. The overall goal is to realign the decision making process for energy efficiency measures in Germanys NRB sector, which is currently dependent on idealism and high investment capabilities.

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<sup>1</sup> Excluding buildings in the sectors industry and transport

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## The CityGML Energy ADE – An International Standardization Effort for the Extension of 3D City **Models to Support Energetic Building Analysis**

Robert Kaden<sup>a</sup>, Mostafa Elfouly<sup>b</sup>, Thomas H. Kolbe<sup>c</sup>

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The current climate and environmental policy efforts require comprehensive planning regarding the modification of the energy supply and infrastructures in cities. Planning comprises e.g. the determination of locations for new power generating facilities like photovoltaic, geothermal and decentralized combined heat and power stations, the widespread introduction e-mobility solutions and hence the of arid development as well as large-scale energetic building rehabilitations. The strategic planning of the different measures requires a holistic approach integrating extensive complex information. In order to establish interoperability between the different planners, stakeholders, and tools, an open information standard is required. In this contribution we will present and

discuss the CityGML Energy ADE, which is a new shared information model for the spatio-semantic representation of the urban structures including energy-related information from different disciplines, based on the international OGC standard CityGML for the representation of semantic 3D City Models. The CityGML Energy ADE is being developed by an international consortium of 11 European organizations, e.g. TUM, TFH Stuttgart, RWTH, KIT, EIFER, CSTB (France), EDF (France), EPFL (Switzerland).

CityGML is an information model and data exchange format defining classes and relations for the most relevant 3D topographic objects (e. g. buildings, transportation infrastructures, city furniture, water bodies) in cities regarding their geometry, topology, semantics, and appearance. The thematic model of CityGML defines classes and attributes e.g. for the semantically decomposed representation of buildings with their thematic surfaces WallSurface, GroundSurface, and RoofSurface as well as for the description of the roof shape, usage type, number of storeys, construction year, and building height. However, energy-specific entities, which are not pre-defined in CityGML are now incorporated using the CityGML Application Domain Extension (ADE) extension mechanism. Due to the rich information model, its extensibility, and the rapidly increasing data availability all over the world, CityGML is a suitable information model for a common engineering data backbone for urban energy, environmental, and mobility planning.

The Energy ADE addresses in its first version all information required to estimate and store building heat energy demands according to different national and international standards like DIN V 18599, ISO 13790, and VDI 3807. 3D building models are enriched by required data. Energy demands can be estimated directly from the enriched building models. The 3D building representation allows to derive required information like surface areas, volumes, shadowing, energy gains by solar irradiation, and thematic data like construction year, number of storeys, and building usage type (e.g. residential or office use). We show how the Energy ADE core model defines thermal building objects by linking them to CityGML classes. A Construction and Materials module covers the construction elements and physical characteristics of buildings. The Energy Systems module represents the relevant building energy indicators, e. g. energy demand and energy consumption, and the energy systems of a building, e. g. conversion and distribution. Additionally, a Building Occupancy module allows for further analysis of demographic changes using census data. It includes the characterization of building usage, ownership and occupancy information.



## **Optimization of carbon nanotubes networks for** organic photovoltaics by ultra-short laser patterning

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Renewable energy has become a much-discussed subject in the last years. With renewable energy sources the emission of CO<sub>2</sub> can be reduced just as the dependence of fossil fuels. Especially, photovoltaics are getting more important, since they enable the consumers to produce electrical power by themselves.

An alternative to long-established inorganic solar cells are organic solar cells. Whether they can be established in the energy market will depend on three factors: Costs, efficiency and lifetime.

One established sort of inorganic solar cells is made of copper-indium-gallium-diselenide (CuInGaSe<sub>2</sub>; CIGS) with a maximum module efficiency of 15.7 %. The advantage of these solar cells is that they are



Figure 1: Produced pattern on a CNT film coated on glass by 400 fs laser pulses at a wavelength of 1030 nm and fluence of 0.27 J/cm<sup>2</sup>

produced as thin-film solar cells and therefore less material is needed. But there are disadvantages too. These solar cells contain indium, which is rare and expensive. Furthermore the CIGS solar cells are produced in an expensive vacuum- and high-temperature-process. Compared to the expensive production of CIGS solar cells, organic solar cells can be manufactured by standard coating and printing

technologies whereby a low-cost roll-to-roll production is possible. Overall the efficiency of organic solar cells (about 3 %) is clearly lower than the efficiency of inorganic solar cells. Besides that, many organic solar cells use also the expensive indium in form of indium tin oxide (ITO) as transparent electrode. But ITO could be replaced by thin carbon nanotube (CNT) films.

To make organic solar cells competitive to inorganic cells, new methods are necessary especially for the increase of efficiency. We present an innovative process to improve the performance of a

transparent CNT electrode film by structuring the thin-film with an ultrafast laser. The transmittance of the electrode is increased by a hole-pattern produced by selective laser structuring of the CNT layer, shown in figure 1. 90

The used sample is 1 mm thick glass substrate with an area of 25 by 25 mm<sup>2</sup> coated with an approx. 40 nm CNT thin-film. The randomly distributed single walled nanotubes with 1/3 metallic and 2/3 semiconducting properties are coated by spray deposition under ambient conditions.

The desired structure is produced by a line-by-line process with highly selective single pulse ablation by 400 fs laser pulses at a wavelength of 1030 nm. The structure consists of holes with 50 µm diameter and 50 µm space between the single holes. Only the CNTs were removed and no damage was found in the underling substrate. By structuring the carbon nanotubes film the transmittance can be increased while the conductivity stays in an acceptable range. With this structure an area ratio of 19.6 % between ablated area and the total area can be adjusted and the transmittance increases from approximately 85 % to 88





% (figure 2) while the sheet resistance increases from 870 Ohm/sq to 1294 Ohm/sq. The results are compared with state of the art ZnO electrode on glass substrate.

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## Metal cluster semiconductor hybrid materials in photocatalysis for chemical energy conversion

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The scarcity of fossil fuels in the near future shows, that more sustainable energy carriers are needed for the future. Metal cluster semiconductor hybrid materials are promosing new composite materials for combined light harvesting and conversion into chemical energy.

The light harvesting is facilitated by the semiconductor where photons with a larger energy than the band gap of the semiconductor produce electron-hole pairs. These charge carriers can be separated and initiate chemical reactions on the surface of the semiconductor. The metalcluster acts as a co-catalysts and takes up charge from the semiconductor, resulting in a more efficient charge separation. In a subsequent step, the separated charges can thus drive chemical reactions such as the hydrogen evolution reaction.

The photochemistry of such systems has attracted considerable attention over the last few years [1,2]. The most explored model system is the photochemical water splitting on such systems, but the yields in hydrogen production are still limited [3]. Another renewable feedstock in this regard is ethanol, since alcohols are the main product from biofermentation and an ideal precursor for biomass in general [4].

However for any reaction, large number of tuning parameters exists (e.g. for the catalyst: the semiconductor, its doping and surface treatment, the material and size of the co-catalyst), which even influence each other. In order to design ideal metal cluster semiconductor systems and to increase the yield in hydrogen production effectively it is of paramount importance to understand the surface chemistry of semiconductor itself under illumination.

To ensure stable and very well defined conditions, we investigate rutile TiO<sub>2</sub>(110). We study those photoreactions with a tuneable dye laser to excite electrons hole pairs. The product analysis is done by quadrupol mass spectrometry (QMS) and the surface composition is monitored via Auger electron spectroscopy (AES). The photochemistry of the system is investigated either by accumulation of photoproduct at liquid N<sub>2</sub> temperature on the surface and consecutive thermal programmed desorption (TPD) or by isothermal experiments monitoring in-situ mass traces of the photo-products.

Exemplified on titania, we demonstrate how the exact mechanisms of photochemical reactions can be elucidated via the judicious choice of the right experimental conditions.

The photochemistry of ethanol on  $TiO_2(110)$  shows photooxidation of the ethanol to acetaldehyde. Although formally 2 hydrogen atoms remain from the stoichiometric reaction equation, no molecular hydrogen is observed. The hydrogen forms water on the surface that poisons the photocatalyst by site-blocking on a defect rich TiO<sub>2</sub>(110) surface [5].

In the last part, we discuss the implications of our findings for metal cluster semiconductor hybrid materials. It has been already shown that the cluster size may play a crucial role in the reaction systems [6].

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## Hybrid thermoelectrics based on a polymernanoparticle composite

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Thermoelectric materials have gained increased attention by the scientific community over the past years due to a high interest in renewable, sustainable and environment-

friendly technologies for energy generation. Thermoelectric devices can be promising for applications such as waste heat recovery in heat engines or as complementary technology to solar cells.

In a thermoelectric material, the application of a temperature difference leads to a change in the distribution of charge carriers through a flux from the hot to the cold side, as seen in Figure 1. The electrical conductivity of the material is therefore a crucial property of the material. Additionally, a sufficiently low thermal conductivity contributes to higher efficiencies. A measure for the usability of a thermoelectric material is the temperature-dependent so-called



figure of merit  $ZT = T\sigma S^2/\kappa$ , where  $\sigma$  describes the electrical with applied temperature gradient. conductivity, S represents the Seebeck coefficient or thermopower of the material and  $\kappa$  the thermal conductivity.

Thermoelectric materials mostly comprise inorganic components, such as bismuth and tellurium. Although these materials show high figures of merit, they suffer from high production costs, energy-intensive nanostructuring steps, and environmental concerns because of potential toxicity of the components and low abundance. In our approach we aim to overcome these problematic factors, which prevent a large-scale application of thermoelectrics, through a novel hybrid approach.

Within this approach we use an organic component, which is the conductive polymer blend PEDOT:PSS. The usage of polymers is especially appealing because of the variability of morphologies, the high availability of such materials and the possibility for solution-based processing under ambient conditions. We combine this organic part with inorganic nanoparticles. The resulting nanostructure shows interesting



thermoelectric properties. We aim for the increase of state-of-the-art ZT values of hybrid thermoelectrics by different means of modification. Treatment of the polymer films with chemical agents allows for a strong increase in electrical conductivity. The introduction of nanoparticles is expected to decrease the thermal conductivity  $\kappa$ , which we are able to measure with the help of free-standing polymer films. Both approaches combined should increase ZT, and thus improve the conversion efficiency.

Figure 2: Conductive polymer blend PEDOT:PSSt

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## Heat Transfer at Supercritical Pressures in Power **Applications – Physics and Experimental Methods**

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Supercritical water is used as the working fluid in modern conventional steam power plants. The unique heat transfer characteristics of supercritical water, caused by large variations of its physical properties near the critical point, have been studied heavily since the middle of the 20th century [1]. The phenomenon of heat transfer deterioration (HDT) at supercritical pressures is of particular importance for the operation and design of supercritical steam power plants. It can cause undesirable peaks in the temperature of evaporator tubes. Figure 1 shows an example of an experimental investigation performed by [2]. The peaks in the measured wall temperature profiles of the evaporator tube are evidence for the occurrence of HDT as the wall heat flux density is increased from 232 kW/m<sup>2</sup> to 384 kW/m<sup>2</sup> at otherwise constant parameters.



Figure 1: Heat Transfer Deterioration in an Evaporator Tube as Observed by [2]

Despite the large number of past investigations, there is still only general understanding of this phenomenon, and a debate on the precise processes that accompany it. The main Disagreements regard the precise (quantitative) definition of HTD, the responsible physical processes that lead to this phenomenon and methods which can be used to predict its occurrence. The latter is especially relevant for the reliable prediction of the behavior of supercritical power plants. In its theoretical part, this study presents the fundamentals and the current knowledge of supercritical heat transfer. It then assesses the definitions for heat transfer deterioration, the prediction methods and the suggested mechanisms found in literature. Comparisons are made amongst the different approaches by use of experimental data from the literature. This leads to the identification of aspects still in need of experimental investigation. In the experimental section, a practical method and a full scale evaporator test rig (HIPER) capable of investigating heat transfer to supercritical water are presented. The test rig has a maximum Power of 1 MW, and can realize steam parameters of 380bar and 580°C. This makes it possible to investigate the aforementioned uncertainties in supercritical heat transfer.

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## **Optimal planning of urban infrastructure networks** for multiple energy carriers

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Current planning of electricity, gas and district heating networks usually happens in separate departments of municipal utilities. The rising use of cogeneration of heat and electricity in a single plant and the growing volatile electricity generation from photovoltaics and windfarms suggests a stronger coupling of the sectors heat and electricity. This research presents a mathematical optimization model for minimum cost planning of hybrid distribution networks with an emphasis on high spatial resolution. The model determines the most economic combination of energy conversion units and transmission lines to satisfy a given distribution of simultaneous heat and electricity demands. Both structure and size of distribution networks are optimized together with size, number and placement of central or local plants. Results are presented for a case study in a small town in Eastern Bavaria. The most sensitive technical and economic parameters are identified to make the difference between different network topologies.



Figure 1: Distribution networks for (from left to right) electricity, heat, natural gas

A mixed-integer linear program (MILP) replicates the planning tasks mathematically. This model is a continued development of a pre-existing model for cost-efficient planning of district heating networks. It features continuous variables for sizing of pipe and plant capacities (in kW), while the decision for building a pipe or plant are modeled as binary (yes/no) variables. Thanks to this formulation, fixed base costs like earth works or minimum installable capacities for plants can be approximated economically without creating many variables. The objective function minimizes total costs for satisfying a fixed given set of energy demands, (here: electricity, heat). Capacities are planned to meet peak loads, while costs are determined based on annual demands. Concurrency effects among energy carriers are respected by empirical prefactors. The model is realized in the programming language Python using the package Pyomo for the model formulation and Pandas for data handling. We use Gurobi to solve the resulting MILP.

Figure 1 shows three optimized distribution networks for a speculative scenario that exhibits several features not common in conventional distribution networks: First, there is only a sparse gas network (right), mainly used for peak heat demand. Second, it features a heating network (middle) that is mainly fed from a central heat pump plant for base load (due to higher assumed COP for a large plant). The electricity grid finally is the backbone for both electricity and heat demand, with many distributed heat pumps for all-year heat demand outside the city center.

In summary, optimization for network planning can support exploring the design space of possible distribution networks to better exploit benefits from coupling heat and electricity.



## Small-scale wind turbine systems with efficient and inexpensive generator topology for micro-grids

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This international cooperation with the University of Stellenbosch, South Africa, is funded by the Bund der Freunde der TUM e.V. The potential use of reluctance synchronous machines (RSM) as generators for small-scale wind turbine systems (≤ 50kW) is examined. Based on a RSM prototype the research tasks at TUM are (i) the design of adequate control and operation management methods and (ii) the evaluation of these developed methods at a Hardware-in-the-loop system at TUM (see Fig. 1).



The evaluation focusses on the comparison of the generator performance of RSM and permanent-magnet synchronous machine with respect to power density, efficiency, dynamics ripple. parallel and torque In these experimental results are used for a further optimization of the machine design of the RSM prototype in Stellenbosch. This talk will introduce and present the project, its goals and first results.

#### Figure 1: Hardware-in-the-loop system

### Advantages of RSM (see [1]-[4])

- Simple and cheap production:
  - Rotor consists of glued and punched iron sheets
  - Expensive permanent-magnets ("rare earth") not necessary
  - Standard stator designs (windings) admissible
- Reliable, compact and efficient machine:
  - Reduced stator and rotor temperature (compared to induction machine) => improved reliability and resilience (e.g. of bearings)
  - Slip rings obsolete
  - Compact design: Re-using the stator design of a 5,5 kW induction machine, the power density was almost doubled to 9 kW at 1500 rpm.
  - High ratios "torque per volume" feasible: 50 kN/m<sup>3</sup> possible (in comparison: permanentmagnet synchronous machines achieve~20-45 kN/m)
- High efficiency (IE4 feasible; at smaller size then standard induction machines)

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# **2** Poster presentations



## Comparison of bottom-up heat demand modelling techniques for residential buildings

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The implications of rapid urbanization on energy consumptions and greenhouse gas emissions post significant challenges to city planners. Holistic urban energy planning, which involves modification of the energy systems to account for the growing share of intermittent renewable energies and energy efficiency improvement through building renovation measures, plays an increasingly important role. Forecasting the energy demand of the residential sector, which represents around a fifth of the total energy consumption in Germany is a key step in the sustainable planning of urban areas.

Space heating constitutes the largest energy use in residential buildings in Europe. A range of heat demand estimation techniques have been developed over the past decades and they can be categorized into topdown and bottom-up approaches. The top-down techniques consider econometric variables and are better suited to analyze the overall supply, while the more complex bottom-up approaches using engineering or statistical methods require more building data for explicit simulations and calculations. For the purpose of planning at larger scale, the latter incorporates spatial attributes from GIS city models, leading to more timeconsuming and complex simulations. Nevertheless, these methods can better meet the needs of an era of fast development of innovative technologies.

As an introduction into further developing a computer model for simulating the heat and electricity demand in cities with fine spatial and temporal resolution, we aim to review different bottom-up techniques for residential buildings to evaluate their accuracy and applicability. The methodology consists of estimating the thermal behavior of typical buildings of the German housing stock using a low-order state-space model of thermal resistances and capacitances (RC) and a complex building energy simulation software. The indoor temperature and energy consumption resulting from the detailed simulation are later fed into the RC-model for parameter fitting. The results of both steps will be finally compared to real consumption measurements in order to analyze the uncertainties, guality of assumptions and limitations.

The comparison aims to reveal the most suitable method to be integrated with a spatial GIS-database and implemented in the energy demand model of the city of Munich. Once completed, the model can be used to evaluate various strategies for climate mitigation, energy saving and urban air quality improvement.



## Novel Catalyst Materials for the Cathode Side of MEAs

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The efficiency of fuel cells is still far below the thermodynamic limit. Due to the high amount of Pt catalyst required to deliver the power needed, especially for automotive applications, the costs are still too high for widespread market introduction. Especially the high overpotential at the cathode side (several hundred mV) due to the sluggish kinetics of the oxygen reduction reaction (ORR) is responsible for these drawbacks. Recently, theoretical and experimental studies have shown that polycrystalline Platinum - rare earth metal (RE) alloys show very promising catalytic properties for ORR, e.g. an increase in the kinetic current density by a factor of 3-5 compared to pure Pt [1,2], and a good stability. The cause of the high activity is the formation of a dense Pt overlayer during the initial de-alloying steps that is under compressive strain [2]. Also, an enhanced mass activity of Pt-RE nanoparticles prepared in a cluster source was reported [3]. The further study of these catalysts and their development towards actual fuel cell applications is at the heart of the FCH JU project "CathCat" that is coordinated by TUM.

The application in real fuel cells requires a method for the production of such nanoparticles, which can be up-scaled to provide enough material for membrane electrode assembly (MEA) fabrication. This is challenging due to the very low standard potentials of the rare earth elements and the resulting sensitivity to moisture and air.

At TUM electrochemical deposition is studied as a scalable method, while other partners focus on solution and gas-phase chemical reduction techniques. Because of the low deposition potential of rare-earth (RE) metals, aqueous electrolytes cannot be used for these experiments. Therefore ionic liquids were chosen as electrolyte, because they offer a wide electrochemical window. In literature a successful deposition of selected pure rare-earth metals had been claimed [4], but there are also reports showing fundamental obstacles for deposition of RE metals from some ionic liquids [5]. In a second approach therefore organic solvents with an added supporting electrolyte were evaluated, which have also a wide potential window and where high amounts of precursors can be dissolved.

For both electrolyte systems, the electrochemical processes in solutions containing Pt precursors, rare earth metal ions and mixtures of both for alloy deposition were studied by various electrochemical techniques, in part in combination with the electrochemical quartz crystal microbalance (EQCM) technique, and ex-situ and in-situ scanning probe microscopy techniques. Aside from the gold electrode of the EQCM, Boron-doped Diamond (BDD) was used as working electrode, as it is a very inert electrode and allows even wider potential windows in non-aqueous media [6]. Deposited layers were characterized by EDX and surface science methods.

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## Characterization of PTB7-Th:PC71BM bulk heterojunction solar cells: The influence of blend ratio

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Traditional fossil fuels as coal, oil and natural gas, play a fundamental role in humankind development since industrial revolution in XVIII century. The success of such fuels lays in the high power density obtainable under combustion and the relative easy extraction process till nowadays. The counterpart of these major advantages is the air, soil and water pollution that their massive use provokes. Moreover, after about two hundred years of huge production these sources are suffering of shortage, difficulties in further supplies exploitation and increasing prices.

In the lasts decades the so called renewable energies, such as wind turbines, photovoltaic cells and geothermal plants reached high impact in unlimited, clean and economically sustainable energy production. The traditional silicon based solar cells are playing a main role in the green energy production conversion, providing the opportunity of small-domestic diffuse plants and ensuring a reasonable payback time. However, the production of such heavy and rigid cells involves rare and/or toxic materials, and is itself high energy-consuming and difficulties arising from the disposal of old cells.



On the other hand, organic solar cells are approaching the efficiency of traditional cells. Moreover, they are promising potentially low-cost and ease production process via roll-toroll printing onto flexible resulting in substrate, а versatile semitransparent cell suitable for innovative design products.

Figure 1: Optical microscope and AFM images of the samples with different ratios

How do the organic bulk heteroiunction cells work? The

cell is like a multilayers sandwich. Each layer has a role in the charges production and extraction, but the crucial part is played by the "active layer". This layer is made by a blend of semiconducting polymer (electron donor, PTB7-Th in this work) and carbon derivate small molecule (acceptor, fullerene, PC71BM in this work). As the light is absorbed an exciton, electron-hole bound couple, is generated in the polymer. In order to harvest the current, the exciton must be split and the charges collected at the electrodes. The fundamental separation process happens at the interface between the acceptor and the donor due to the electric field built up by the different materials work function. Thus, the morphology of the active layer plays an essential role in successful cells.

In this work five samples with different ratios between polymer and fullerene have been prepared. The optical proprieties of the films have been measured via UV-Vis absorbance, testing the ability of absorbing light; and via photoluminescence response in order to measure the number of excitons effectively separated in each film. The surface morphology has been overviewed with optical microscope and observed up to nanometer scale with atomic force microscope (AFM). The inner films morphology has been examined by grazing incidence small angle X-ray scattering (GISAXS). The information about the vertical material composition has been extracted via X-ray reflectivity and a deeper sight into crystalline structure has been given via grazing incidence wide angle X-ray scattering (GIWAXS). Finally, solar cells have been fabricated out of the five ratios. Their performances have been tested under solar simulator measuring current-voltage curves and obtaining out of these the electrical parameters for each device. Moreover, the external quantum efficiency (EQE) of the cells has been measured enabling to know how many electrons are collected for each wavelength of the solar spectrum.



### Novel nanostructured thermoelectric materials

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The performance of thermoelectric materials is defined by the figure of merit containing the squared Seebeck coefficient multiplied with the total electric conductivity devided by the total thermal conductivity. These properties could be changed in various ways, e.g by manipulation of the crystal structure, doping or participation formation and particle size.

For our collaborative project 'Novel Nanostructured Thermoelectric Hybrid Materials' between the groups of Prof. Dr. P. Müller Buschbaum (Physics), Prof. Dr. M. Brandt (WSI) we examine Ag<sub>10</sub>Te<sub>4</sub>Br<sub>3</sub> and AgBiSe<sub>2</sub> due to their extraordinary thermoelectric feature like reversible p-n-p switching upon structural phase transitions [1, 2]. In the case of  $Ag_{10}Te_4Br_3$  a thermopower drop of 1400 µV K<sup>-1</sup> was measured at around 390 K. Via substitution of the halide ions this value can be maximized to more than 3000 µV K<sup>-1</sup>.

It is planned to use such materials to fabricate nanostructured hybrid thermoelectrics using state of the art conductive polymers.



DSC data for Ag<sub>10</sub>Te<sub>4</sub>Br<sub>3</sub>. [1]

On the other hand it is well known that multiscale-disorder such as pores, grain boundaries and inclusions can reduce the thermal conductivity drastically.

Using pulsed laser sintering (LS), thin films of Si or Ge nanoparticle with a mesoporous semiconducting network could already be achieved [3]. We have applied this advanced LS technique to Ag<sub>10</sub>Te<sub>4</sub>Br<sub>3</sub> and AgBiSe<sub>2</sub> to fabricate comparable thin-films. Through ball-milling or high-shear mixing a particle size of around one hundred nanometers could be obtained. This size is sufficient to realize suspensions for spin coating. Laser sintering of the obtained thin films lead to the typical mesoporous network as for Si or Ge nanoparticles. We intend to characterize such thin-film arrangements and intend to prepare hybrids in the near future.



Figure 2: SEM of LS thin films of AgBiSe<sub>2</sub> showing a meander-like structure and porosity.

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## Low-Tech solutions for electric power supply in Nepal

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Challenges: Lack of energy is often the reason for extreme poverty and hinders progress in developing countries. Worldwide, 1.5 billion people have no access to electrical energy. In Nepal this is the case for 15 million people (50 % of the population). The other half of the population is affected by power cuts, which



often last for 16 hours per day. The scarcity of electrical energy is will vastly increase in the near future. While the Earth's population grew by 16 % between 2000 and 2013, their energy consumption increased by 31 %. In developing countries, the energy consumption climbed even faster: by 70 % during this period.

Chances: While the energy consumption in developing countries is vastly increasing, they hold huge potentials for renewable energy production. Nepal for a example has one of the biggest hydro energy resources found anywhere on Earth: experts estimate the technically extractable potential to around 40.000 megawatts. So far, less than two percent of this energy is used. With adequate technologies, this number can be raised in order to strengthen sustainable progress in developing countries.

Key factors: Figure 1 illustrates five key factors that are important for a successful implementation of the project. In order to find a technology for electric power supply that suits the social, cultural, economic and ecological circumstances in remote regions of Nepal, surveys with intensive discussions and questionnaires were done with local people. By working out a corporate project plan that involves the needs and ideas of domestic people, transferability to other communities is maximized.

230 Volt water wheels: Water wheels are deployed as small-scale hydropower stations in order to supply remote areas in Nepal with electric energy.

The first prototype has been installed in 2014 in the Solu Khumbu region in East-Nepal. Apart from the asynchronous motor / generator, all parts for the 230 V alternating current power station were bought locally. A key aspect of the project is the empowering approach: local people shall learn how they can help themselves and each other. Therefore, water wheel was constructed in close the collaboration local people. The goal of the water wheel project is to supply three to five families with uninterrupted 230 V alternating power.

5 Volt USB water wheels: This really small water wheels with a 5 V USB Hub can be used for charging mobile or for small lighting.



Figure 2: water wheel prototype in Nepal

Implementation: By empowering local people to build their own means of electric power supply, local resources are exploited and a sustainable development is initiated. Technology transfer and scientific insights are multiplied by teaching local project coordinators who will be able to build and repair power plants in the near future with only minor input from abroad.

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## Zintl Clusters as wet chemical precursors for inverse opal structured germanium/silicon morphologies for photovoltaic applications

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We present a versatile wet chemical method utilizing homo- and heteroatomic  $[E_9]^{4-}$  (E = Si/Ge) Zintl clusters for the fabrication of inverse opal structured germanium/silicon films as well as results on the application of such materials in hybrid solar cells with poly(3-hexylthiophen-2,5-diyl) (P3HT) as hole conducting polymer.<sup>[1]</sup>

Ordered porous inorganic semiconductor morphologies are proven to be valuable for the fabrication of



efficient hybrid solar cells, due to high interface areas for efficient exciton dissociation and continuous pathways for the charge transport.<sup>[2]</sup> Silicon and germanium, instead of widely used metal oxides, are in particular interesting due to their broad adjustability of optoelectronic properties, e.g. by nanostructuring and/or preparation of solid solutions Si<sub>x</sub>Ge<sub>1-x</sub>, combined with high charge carrier mobility. However, the majority of fabrication methods for such germanium/silicon morphologies are elaborating and ground on complicated physicochemical techniques, owing to the lack of precursors suitable for wet chemical reactions.<sup>[3]</sup>

Figure 1: SEM micrographs of inverse opal structured Ge (left) and Ge/Si (right) films fabricated by the presented method.

We found a facile method to utilize homo- and heteroatomic  $[E_9]^{4-}$  Zintl clusters as flexible wet chemical precursors for the fabrication of germanium/silicon morphologies, which can be applied by drop casting and spin coating on substrates or template structures, respectively. The clusters are crosslinked with group 13-15 halogenides  $E'X_n$  (E' = B, Ge, Si, P; X = Cl,

Br; n = 3.4) giving elemental E/E' and enabling the introduction of dopants like boron or phosphorous, respectively. The potential of our method is demonstrated with the fabrication of inverse opal structured germanium/silicon films. The films were characterized with respect to their morphology and chemical composition by electronmicroscopic and spectroscopic methods. Moreover grazing incidence small angle scattering (GISAXS) was performed with an amorphous inverse opal structured germanium film, to get insights in the volume morphology.

Hybrid solar cells were assembled by fabrication of inverse opal structured films on FTO/TiO<sub>2</sub> and filling of the pores with P3HT.

# FTO TiO<sub>2</sub> РЗНТ Au

Figure 2: Assembled type of hybrid solar cells used for testing the inverse opal structured films.

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## Impact of Water on CO<sub>2</sub> Adsorption of Amino-**Functionalized Hierarchical Silica Spheres**

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Due to the constant increase in worldwide energy consumption, much of which is satiated by the use of fossil fuels, atmospheric CO<sub>2</sub> levels have been rising for decades. To stop this trend, effective means to remove CO<sub>2</sub> from flue gas streams are required. The benchmark process is absorption in aqueous amine solutions, which features high selectivity towards CO<sub>2</sub>. However, its efficiency is limited by the high heat capacity of water, which makes regeneration heavily energy demanding.<sup>1</sup> Furthermore, leaching of amines occurs at elevated temperatures. Thus, amine-functionalized silica materials are widely investigated as sorption materials due to their lower heat capacity, tunable surface areas and possibility to chemically tether the amines to the support. While adsorption under dry conditions is widely investigated, the influence of



Figure 1: Possible adsorbed species

water, which is typically present in flue gas streams, on adsorption warrants research.

The influence of water on the CO2 adsorption of amine-functionalized macroscopic silica spheres with hierarchical pore systems was investigated. The materials were synthesized in a one-step, surfactant-templated, emulsion based synthesis. Various aminesilanes were used for functionalization. Sorbents were consequently characterized using nitrogen physisorption at 77K and elemental analysis. Adsorption of CO<sub>2</sub> at 50°C was followed using thermogravimetric analysis coupled with differential scanning calorimetry. <sup>13</sup>C MAS-NMR and IR spectroscopy were used to characterize the interaction between CO<sub>2</sub> and the functional groups of the sorbents.

The adsorption of CO<sub>2</sub> on amines leads to different species depending on the type of amines and the presence or absence of H<sub>2</sub>O on the sorbent (Figure 1). Under dry conditions, mainly carbamates

are formed. This anion has to be stabilized by a neighboring cation, which is created by the protonation of a second amino group. In vacuum, we found carbamic acid additionally to carbamate for secondary amino groups. It also has to be stabilized by a second, protonated amino group, leading to a maximum 2:1 stoichiometry of amino groups to  $CO_2$  under these conditions. In the presence of water,  $CO_2$  can be adsorbed in the form of (bi-)carbonates as well as surface bound carbamates. For these cases, stabilization with one amino group is sufficient per molecule of CO2, leading to a 0.4maximum stoichiometry of 1:1.

A comparison of two CO<sub>2</sub> adsorption isotherms at pressures between 0.3 and 100 mbar under dry and pre-hydrated conditions is shown in The corresponding spheres were functionalized with Figure 2. approximately 2 mmol/g of a secondary aminesilane (N-methylaminopropyltrimethoxysilane, MAPS). The uptake capacity under dry conditions is considerably lower than the theoretical maximum of 1 mmol/g, which can partly be attributed to the steric restraints of secondary compared to primary amines.<sup>2</sup> It decreases even further if the spheres are hydrated, despite the proposed change in mechanism leading to a 1:1 stoichiometry. However, the expected increase in uptake



### adsorption isotherms

capacities was found for amine-impregnated SBA-15 materials. We thus assume that the co-adsorption of H<sub>2</sub>O and CO<sub>2</sub> on inner adsorption sites and condensation of water in the smaller pores of the hierarchic system lead to a decrease in accessible sites for CO<sub>2</sub> sorption. While the hierarchical pore system has been found to be beneficial for temperature-induced regeneration of sorbents, it thus needs to be tailored to ensure pore sizes above the limit for pore condensation of  $H_2O$ . [1] D.J. Fauth, M.L. Gray, H.W. Pennline, Energy Fuels 2012, 26, 2483-2496

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## Investigations on ZnO 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 make the device - depending on the substrate - transparent and flexible. Moreover, the producing is less energy demanding. These properties hold new possibilities in energy saving, e.g. for room lighting.

scattering layer

The research was mainly focused on the internal quantum efficiency to enhance the conversion of electrical power into light which makes the OLED 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 absorbed eventually.

Hence, there is still a high potential for the enhancement of OLED efficiencies by increasing the photon extraction.

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 structurefunction relationship.



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## Window machine

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External wall constructions and thermal glazing have been optimized over the years to the extent that they exhibit excellent thermal performance. The weak point in wall systems is now the junction between the window frame and the wall and insulation.

This research project at the Chair of Building Construction and Material Science of the TU Munich investigates how a range of related requirements can be incorporated into a multi-functional window element. By including solar shading and glare reduction elements, intruder protection, ventilation with heat exchanger and electrification / automation technology in a prefabricated unit that is also attractively designed, the "window machine" aims to improve the quality and performance of the building, while being quicker and easier to install at a lower cost

Our research focuses on the energetic refurbishment of buildings of the 1950s until the 1970s. Selected on a modular system, the technical elements can be incorporated into every unit. They can be chosen from the beginning or be upgraded later on. As a key feature the different alternatives integrate various concepts of heat (and humidity) recovery ventilation without requiring additional penetration of the wall.



Figure 1: models of three investigated alternatives

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## Assessment of energy-related refurbishment strategies via Bayesian-Network modelling

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Task/ State of the art: Portfolio managers, building owners, public institutions or real estate companies increasingly ask for economic and efficient ways to develop holistic refurbishment strategies to efficiently modernise their building stock. The highlighting of necessary refurbishment measures, the selection of buildings that have a certain energy-saving potential or a weak-point analysis of the building stock are only



Figure 1: Bayesian Network, window replacement

a few of the requested features a potential tool should provide. Several studies and databases focus on these questions and offer a wide overview over various building age classes, including typical construction characteristics, agespecific weaknesses and potentials, which result in general modernisation measures and energy-saving potentials. What is not taken into account are the uncertainties of databases which just cover a small scope of various building, due to the big amount of variation in the building stock. Thus the indication that buildings, for example built before 1918, have windows without any insulation and therefore a replacement should be the first measure in saving energy, is just a

likelihood, representing the "experience of the database" and of undertaken measures. Methodology: In order to reflect the existing uncertainties in recommending refurbishment strategies, a probabilistic approach have to be chosen. In the proposed project a Bayesian-Network (BN) has been implemented in the process of ranking suitable modernisation measures related to their economic and ecological consequences. BNs combine principles from graph theory, probability theory, computer science, and statistics. The graphical structures in the elaborated model, like for instance in Figure 1, are used to represent knowledge about an uncertain domain (building construction and condition). In particular, each node in the graph represents a random variable, while the edges between the nodes represent probabilistic dependencies among the corresponding random variables (condition of windows, opague elements etc.).

Case Study: The probabilistic model will be filled with data of existing refurbishment projects and implemented and validated on the building stock of the Ludwigs-Maximilians-Universität (LMU, Figure 2)) Munich. The associated research program HoEff-CIM focuses on automated and eased energy efficient refurbishment of universities and colleges. Thus the LMU will get deep knowledge of the likelihoods of costs and energy saving potentials of specific refurbishment measures for specific building types and ages.

Expected Results/ Outlook: The Bayesian network model will deliver several outputs. Primary it will indicate which refurbishment measures imply which energy saving potential and generated costs. It will help

to identify the most reliable, sustainable and cost effective measure and provide an overview over the risks and uncertainties induced by the inevitable assumptions and calculations related to existing buildings. It will be a powerful tool to help decision makers to estimate the impact of building refurbishment measures even before entering and inspecting the building. In combination with a quick check tool for rapid building survey, actual energy consumption data and building simulation the Bayesian-Network-model is able to create efficient and sustainable modernisation strategies for various building types and usages.



Figure 2: thermography of a case study building

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## **Resonant Grazing Incident Small Angle** X-ray Scattering of Conducting Polymers

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In recent years the use of X-rays for investigations on the morphology of polymeric thin films in photovoltaics has increased. X-rays are a suitable tool to investigate morphological changes in polymer films. Generally hard x-rays around 10 keV are used to probe organic photovoltaic samples in grazing incidence geometry. While this energy is suitable for strong changes in electron density as can be found in mixtures of standard organic photovoltaic materials (polymer/fullerene), there are much less changes in the electron density for polymer-polymer systems and therefore much lower scattering contrast.

However, it is possible to analyze such latter systems by choosing x-ray energies in the vicinity of absorption edges of certain elements. This method is called resonant scattering. In previous works it has been shown that measuring at the absorption edge offers the possibility to distinguish two polymeric components from each other and hence offering the opportunity to analyze the morphology of such a system. [1, 2] The quoted work has been carried out at energies of the 1s absorption edge of carbon as carbon is a common element in every organic molecule.

The focus in the presented work is the examination of the influence of the morphology of a P3HT: PCBM blend induced through a second non-conducting polymer. Understanding the changes in the morphology requires a suitable method to distinguish the two polymers from each other. The notable, chemical difference between the two polymers is the sulfur present in the semiconductor but not in the nonconducting polymer. Exploiting the energies around the sulfur edge offers the possibility to concentrate on the contrast between the non-sulfur containing components to the sulfur-containing P3HT. The polymer films are thin (around 100 nm) which decreases the scattering volume in a transmission geometry. Therefore it is necessary to combine the strength of the resonant scattering with the volume probing characteristics of the grazing incident small angle X-ray scattering (GISAXS) technique. GISAXS measurements at the sulfur K-edge were performed at the four-crystal monochromator beamline of PTB at BESSY II using an in-vacuum Pilatus detector. Probing the samples with the combination of these two techniques results in a strong energy dependency of the scattering patterns. This information is used to gain information on the inner film morphology of the studied ternary system.

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## State feedback control and observer design of gridconnected power inverters with LCL-filter

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More and more electrical systems are connected via power electronics to the electrical grid. The use of grid-connected voltage source power converters allows for independent control of active and reactive power exchanged with the grid. However, in power generation systems like wind turbine and photovoltaic systems, the ability to meet grid codes becomes more and more important for a stable grid operation. Therefore, in view of the switching nature of the power electronics, filters for the grid connection have to be used. A particularly cost-efficient and high-



Fig. 1: Grid-connected voltage source converter with LCL-filter

performance solution for medium-size renewable energy systems is the LCL filter. Its drawback is its resonance frequency which makes damping essential for a stable operation. To assure a stable and welldamped operation, in this poster we propose a state-feedback current controller with Luenberger observer and additional 1) compensation of the converter dead time, 2) grid voltage feedforward control/compensation (GVFC) and 3) filter current decoupling control (FCDC).



Fig. 2: Block diagram of the three-phase system

Fig. 1 shows the three-phase system with DC-link voltage, voltage source converter, LCL filter (with converterside inductance & resistance, filter capacitance & resistance and grid-side inductance & resistance) and the symmetrical (ideal) grid. Control objective is grid-side current tracking to allow for independent active and reactive power control at the point of common coupling (PCC). To reduce the number of sensors, we allow only for converter-side current and grid

voltage measurements, which necessitates the design of a state observer. Fig. 2 shows the block diagram of the three-phase system with pulse-width modulation (PWM) as modulation scheme for the voltage source converter plus the implementation of controller and observer (with additional Clarke- & Park transformation and phase-locked loop (PLL)).

Besides the modeling of the three-phase system and the controller & observer design, the poster demonstrates the system behavior, the controller & observer performance plus the effects of GVFC and FCDC via simulation results (Matlab/Simulink). Also parameter sensitivity of controller and observer are illustrated. It is pointed out that the designed controller & observer guarantees a stable and well-damped operation. Even for parameter deviations between system and controller & observer, an acceptable reference tracking performance of the grid-side current is achieved.


### Thermal behavior of Li-ion cells - an in situ neutron diffraction study

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Among various approaches towards battery development, the in situ characterization of the entire battery system during electrochemical cycling is the most promising one. This type of experiment on cells from serial production must be non-destructive, where all materials of the battery remain under real operating conditions and any risks of their changes are eliminated. For this purpose neutron scattering is well-suited tool and high-resolution neutron powder diffraction shows excellent performance when changes on nanometer scale are intended to be observed [1, 2].



The behavior of commercial 18650-type cell (LiCoO<sub>2</sub> cathode and graphite anode; 2600 mAh, 3.0 - 4.2 V) in a broad range of temperatures (150 K - 368 K) was investigated in situ using combined high-resolution neutron powder diffraction and electrochemical analysis. The Rietveld refinement technique was applied for structural characterization of the electrode materials in discharged and fully charged states of the cell as a function of temperature [3].

The performance of the cell drops drastically at a temperatures below 250 K, while further heating leads to an improvement of its characteristics and an increase of the nominal cell capacity (Fig. 1).

Figure 1. Temperature dependence of Li-ion cell capacity.

Structural details of both positive and negative electrodes as well as their thermal evolution were experimentally investigated. The influence of elevated temperatures on the anode is reflected in higher graphite lithiation observed by formation of an additional amount of stage I - LiC<sub>6</sub>, which is consistent with the increased cell capacity (Fig. 2).



A steady increase of lattice parameters a and c in LiCoO<sub>2</sub> cathode was observed upon stepwise heating of the cell. Thermal expansion of LiCoO<sub>2</sub> has been found strongly dependent on the lithium content, which can be attributed to the weakening of bonds between neighboring CoO<sub>2</sub> layers upon lithium removal.

The analysis of the Li occupation in Li<sub>x</sub>CoO<sub>2</sub> in two extreme states of charge reveals an increase of the "active" lithium amount taking part in a charge transport at elevated temperatures. Differences in lithiation of cathode and anode upon cooling of the charged cell were observed, which might be important for the further optimization of battery cycling conditions.

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## **Polymer-Based Solar Thermal Drain Back Systems**

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The ongoing public debate on the future of energy supply in Germany is often reduced to the question of renewable electricity generation. Considering the percentage of energy consumption in private households in Germany, it is found that almost 85 % of the energy is required in the form of heat (Figure 1). Despite the



Figure 1: Energy consumption in private households in Germany in 2013<sup>1</sup>

sophisticated systems, solar thermal energy accounts for only 1 % of residential heat demand in Germany in 2013<sup>2</sup>. To increase the share of solar thermal heat used in residential buildings, the costs of solar thermal systems must be reduced to achieve a competitive advantage over other heat sources. In this context, polymers offer a large cost saving potential. The positive engineering properties of plastics such as low weight, freedom of design and manufacturing techniques have contributed to the success of these materials.

Integrating polymeric collectors into standard solar-thermal systems offers only limited economic benefit, because reduced collector costs alone cannot compensate the decreased efficiency of such setup. High temperature, high system pressure and the UV-irradiation represent further challenges for the application of polymers in solar thermal systems.

As a consequence, new systems are required which take the specific properties of polymeric solar thermal collectors into account. The open, unpressurised architecture of drain back systems (Figure 2) is able to meet the requirements of polymers and allows a wide application of polymers in other parts of the solar circuit. Compared to conventional solar thermal systems, the biggest advantage of a drain back system is the overheating and freezing protection, which enables the usage of water as the heat carrier. On the other hand, higher installation and operating costs may limit the economic benefit of these systems.

This research project aims to develop a cost-effective solar thermal drain back system with polymeric collectors. In this context, measurements as well as simulation studies will be performed to evaluate the benefit of such a systems. In a first step, different types of drain back systems were categorized with regard to their suitability in combination with polymeric materials. The manufacturing and installation costs of these systems as well as their energy demand were taken into account. We identified five different types of drain back systems, with two systems being especially promising for a combination with polymeric materials. In the next step, the energy demand for the pump will be evaluated regarding the installation position of the drain back volume.



Figure 2: Scheme of a drain back system

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### Influence of drying dynamics on performance of printed organic solar cells

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State of the art solar cells are currently made of silicon. Its processing, however, requires a lot of energy. A promising alternative are organic solar cells. They exhibit the advantage of high absorption and therefore a low amount of material is needed for the production. Furthermore, latter ones can be processed out of



Figure 1: Setup of a typical organic solar cell and working principle in an energy diagram

solution. This offers the possibility for large scale production via coating and printing techniques like knife coating, slot-die coating, screen printing or spray coating. [1] Typically, the active layer of an organic solar cell is sandwiched between two electrodes (Figure 1). An blocking additional layer prevents charges from recombining at the wrong electrode. The active layer absorbs the light and consists of two materials. In the energy diagram in Figure 1, the working principle of organic solar cells is shown. Incoming light is absorbed in the socalled donor and an electron is excited into a higher energy state (I) but still bound with the remaining hole. The bound charges diffuse to an interface (II),

where the electron is transferred to the acceptor material (III). The separated charge carriers are then extracted via the respective electrodes (IV and V).

Currently, the most common method to produce organic solar cells is spin coating, which is intensively studied. It is known, that by varying the solidification time after spin coating, the performance of the produced devices can be optimized. [2] However, using spin coating upscaling to an industrial process is

not possible. The knowledge gained from spin coated samples cannot easily be transferred to other coating techniques as they differ in the kinetics and dynamics of film solidification. [3]

In this study, we investigate the influence of the drying dynamics on the performance of printed organic solar cells. The films are characterized using optical microscopy and UV-Vis spectroscopy. Figure 2 shows the homogeneity of the printed active layer. The I-V curves of the obtained solar cell devices show the influence of different drying conditions on the device performance. This work helps to further understand and optimize the production routine of printed organic solar cells.

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### Mesoporous germanium morphologies with inverse opal structure as anodes for 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.<sup>[1]</sup> However, these materials suffer from tremendous volume changes during cycling which is the dominant obstacle for its practical use. Herein we report a synthetic strategy for the preparation of mesoporous undoped and P-doped germanium thin films to overcome the mechanical difficulties of such electrodes. Our synthetic strategy bases on controlled oxidative decomposition of Zintl clusters in presence of a

template structure and an optional phosphorus donating precursor compound. Concretely, we succeeded to prepare and dope mesoporous germanium films with inverse opal structure assembled from K4Ge9 Zintl clusters using a wet-chemical method utilizing triphenylphosphine or sodium heptaphosphide as P sources. Morphological analysis of the obtained films by scanning electron microscopy (SEM) displays the formation of ordered mesoporous networks independently of the applied dopant. Fano interference in Raman spectra evidence successful doping. Increasing electrical conductivities further support successful phosphorous doping. First electrochemical studies show promising cycle performance and rate capability.



## **Bringing Distributed Energy Resources to Market**

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The integration of non-dispatchable generation from renewable energy resources with random power output, in particular wind and solar, requires a paradigm shift from load-following supply to supply-following load. Distributed energy resources (DERs), such as electric vehicles (EVs), heating, ventilation, and air conditioning (HVAC) systems, and stationary battery energy storage, can be controlled to shift load on different time scales without compromising their primary use. Controlling DERs using information and communication technology (ICT) could turn out to be more flexible and less expensive than deploying dedicated centralized energy storage, but is to some extent restricted by dynamic user behavior. Their fast response capability and spatial distribution makes DERs ideal candidates for addressing various renewable integration challenges. They can help to improve voltage quality in distribution feeders and reduce the peak-to-average ratio of power demand, thereby enabling a more efficient use of existing power grid assets. They can also be used to supply balancing power, which is needed to guarantee the secure operation of power systems. To realize this potential, academia and industry have to address challenging issues, including the technical and economical evaluation of these resources, the exploration of new control and optimization techniques, and the development and evaluation of ICT systems that meet the requirements imposed by the control task. In addition to executing the control task including all required communication, optimization and input/output, such systems have to be highly reliable and scalable.

This poster will present our latest research results on supplying balancing power using distributed battery energy storage and EVs. We are particularly interested in scenarios where aggregators control these resources directly to participate in existing power markets. This turns out to be a highly demanding task, both from the communication and optimization point of view. We evaluate the potential of market participation scenarios, propose pragmatic control and optimization techniques, and outline the vision of advanced ICT systems that could help to realize scalable and reliable resource control. Our evaluations are based on actual operational processes of power system operators, power market data, renewable power generation data, and simulations of dynamic resource behavior, e.g., driving patterns of vehicles.



### Performance of P3HT:PCBM organic solar cells doped with iron oxide(II,III) nanoparticles

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Organic solar cells are an interesting alternative to conventional silicon based solar cells as the feature new possibilities introduced by using a different class of materials namely polymers. Instead of expensive ultrahigh vacuum technologies, fabrication can be done by room temperature, wet chemical processing, and thereby enabling usage of methods such as roll-to-roll printing. As a consequence, the production of organic solar cells has the potential to become very cheap and easy. Moreover, the use of polymers allows for flexible solar cells and light weight devices, which will be usable in a very different fashion as compared to the immobile silicon solar panels. In addition, the energy payback times of organic solar cells are significantly shorter as compared to the today's silicon solar cells. However, despite all these significant advantages of organic solar cells, still some problems need to be overcome to render them ready for successful commercialization.



Figure 1: GIWAXS detector data file with the most prominent P3HT families indicated in red and in green, depending on their orientation with respect to the sample substrate. PCBM ring is highlighted in black.

Among the different systems studied in organic solar cells, the combination of poly(3hexylthiophene) (P3HT) and [6,6]-phenyl-C60butyric acid methyl ester (PCBM) has received the highest attention due to easy commercial availability. However, regarding a further boost in efficiencies doping with heavy metals has shown interesting behaviors.



respectively.

Figure 2: Lab- produced organic solar cell on a glass substrate

The morphology is probed with advanced scattering techniques (see figure 1)

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## Non-Intrusive Load Monitoring and Data Disaggregation

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The shift from fossil fuels to green energy has increased the importance of effective energy monitoring techniques to efficiently manage the use of electricity. Usually smart meters, capable of bi-directional communication and power transfer, are deployed for measuring the overall energy consumed in a household. In order to achieve effective consumer participation, overall energy consumption information is usually not enough. Some studies have indicated that considerable savings can be achieved by sharing real-time, fine-grained energy consumption information at device level with the consumers instead of other indicators, like monthly bills and electricity usage advice. To achieve these objectives, two approaches namely intrusive load monitoring (ILM) and non-intrusive load monitoring (NILM) are commonly utilized. The NILM approach has gained wide popularity due to its ease of installation and management. Apart from increased privacy and reduced cost, as compared to the ILM or other traditional approaches, the main advantage of NILM is the single point for sensing consumption information (i.e., at electricity mains). Later the load data can be disaggregated to identify individual appliances, determine energy wastage and even detect the faulty appliances from its characteristic curve. One of the limiting factors of this approach is the lack of high-resolution data sets for reliable load data disaggregation.

This work primarily addresses the issue of reducing the uncertainty resulting from the application of different disaggregation algorithms. The idea is to acquire data at an adequate rate (high frequency) to get a highresolution digital image of the analog input, which when fed into different data disaggregation algorithms, helps boost their overall performance. This also helps the feature extraction (load signature extraction) process and ultimately leads to better load identification due to reduced uncertainty. The consumer behavior differs significantly but plays an important role in any energy-monitoring algorithm, especially with regards to prediction and disaggregation schemes.

The origins of uncertainty to acquire high-resolution image stem from the analog to digital converter (ADC) and current transformer (CT). Majority of off the shelf energy monitors are equipped with 10-bit or less ADC, which can serve well for the low frequency analysis but are not adequate for high frequency analysis. In our

experimental setup shown in figure 1, we have utilized a USB sound card along with software oscilloscope for real-time energy measurement and storage. The use of sound card as ADC has shown promising results in terms of high resolution thus helping to detect even lower rated devices and have eased the feature extraction process for individual loads. Our ultimate goal is to combine all these features into all in one solution for the next generation of low cost, high frequency smart energy meters capable of NILM and remote appliance switching.



Figure 1: Use of sound card as energy monitor

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# Cheap water treatment for developing countries

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Water supply is increasingly becoming a problem in poor countries. 750 million people around the world lack access to safe water. Rich nations can afford expensive water treatment, whereas poor countries cannot. Various projects to improve water quality for development countries have failed either at the cost or the lack of userfriendliness. We are trying to eliminate these problems with decentralized cheap water treatment plants.



#### The construction:

Two different large PET bottles are needed per cascade for the water treatment plant. The bottoms of the large bottles are cut off so that they can stick to each other. The distillate water is collected from the underside of the large bottles. The small bottles, in which the dirty water flows, are cut lengthwise. The system is mounted on the roof and filled with dirty water once a day.

#### How does it work:

The dirty water is first cleaned by a simple biological sand and gravel filter and then it runs in the 2-chamber container. On the one hand the water is distilled by the sun and on the other hand, it is disinfected by the UV radiation. The bottles are also used here as a sedimentation tank and thus, the impurities in the water can settle on the ground. In the distillation process all toxic residue such as cyanides, arsenic, lead, zinc, chromium and mercury can be removed from the water. After that, the water is safe to drink, especially for new-borns, clean drinking water is very important.

In combination with UV disinfection, all pathogens that couldn't be removed by distillation get killed. The water treatment plant uses the disinfecting effect of UV-A light (wavelength 320-440 nm) to its advantages. Pathogens (diarrhoea, cholera, etc.) are largely destroyed by sufficient long sun irradiation. At temperatures above 50°C, a strong synergistic effect of UV-A radiation and heat can be observed, which further increases efficiency.



Based on evaporation levels of 8.8 litres per square meter (average solar irradiation in Casablanca, Morocco), one bottle (25 cm long and 10 cm wide) yields between 0.22 litres of condensed water and 1.0 litre of disinfected water per day. Six bottles in a row would cover the daily requirement of fresh water for a child.

#### Why is this innovative?

1. Easy to use: There are already simple methods for water purification but unfortunately, they are either expensive or impractical. Because of the cascade design, the system must be filled only once a day and provides constant purified water.

2. Enough water for daily requirement: The main goal is the production of sufficient water for a family, what can be achieved through the production of drinking and service water. On the one hand absolutely clean drinking water is produced on the other hand, sufficient amounts of disinfected service water.

3. Very Low costs by using local available material: The simple bottle construction is very cheap and easy to produce. Furthermore, no high investment costs are necessary. The required PET bottles are available worldwide and there is no need for maintenance engineers. Broken or turbid bottles can be exchanged easily and without problems by the plug principle.

The current research is mainly the cost reduction, development of simple construction and empirical evidence on the effectiveness of the system. The right of access to clean water has been recognized on 28 July 2010 by the General Assembly of the United Nations as a human right. It's time to implement this human right.

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## **Development of a Raw Material Model for Urban** Districts

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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].

One major aim of this project is to identify what types of materials and how much are contained in different residential building types. This inventory sets the basis for analysing the raw material flows over the whole live cycle of urban districts. The life cycle approach can give an indication at what times raw materials are required (e.g. insulation for retrofit measures), and when raw materials become available again, for recycling or disposal, after the end of life of individual components of the district.

The developed raw material cadastre can then be integrated into GIS systems 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 district as a whole. Due to retrofit-, new construction- and demolition measures, the overall energy consumption of the district during the use phase will be reduced, as higher energetic building standards are being achieved through these measures. However, energy (embodied energy) and other raw materials will also be required to produce, deliver, recycle and dispose of the individual building materials that flow into and out of the urban system. As the individual material flows (live 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<sub>2</sub> emissions) the individual measures may have.

This integrated approach is not only examining the live 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 of these systems. 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 [2].

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#### **Renewable Energies in Quarters - Energy Efficiency Potentials of Low-temperature District Heating Networks**

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The increasing interconnection of energy demand and energy supply promotes the integration of renewable energy sources and further utilization of energy efficiency potentials. Low-temperature district heating networks offer significant advantages on the side of energy supply: absorption of renewable low-grade heat, reduction of thermal losses and optimization of the overall energy efficiency of the system through the temporal and spacial shift of heat within the district.

Prerequisite for the utilization of these benefits is a fundamental understanding of the limits of this technology, the framework conditions of use, the economic efficiency and the operational interdependences during the use of the grid. On the basis of an exemplary district with urban density the research project analyzes: heat demand limits, storage capacity and seasonal use of grid and storage, as well as the profitability of the low-temperature district heating networks.

Preliminary investigations considering the requirements of said exemplary district and of the technologies applied, led to the design of a low-temperature district heating network with seasonal storage, PVTcollectors and decentralized heat pumps. The design aims for maximizing the energy output while minimizing the input of non-renewable primary energy. Based on the network design a TRNSYS model is built which simulates the thermodynamic behavior of the network (Figure 1). First simulation runs indicate a strong interdependence of network temperature, seasonal storage volume and energy efficiency of the heat pumps. With an increasing amount of thermal mass in grid and seasonal storage, a higher system efficiency as well as a more robust system can be achieved. Another important influence on the system efficiency is the required pumping power. The increase in flow needed during the summer months to cool the PVT collectors and charge the seasonal storage allows for an efficient use of the electricity on site, also produced by the PVT collectors.

Further research tasks will be the refinement of the simulation model and the examination of the profitability of the system as well as the suitability of different heat storage technologies. Goal of the project is to enable a broader use of local energy potentials such as solar irradiation and waste heat in buildings. Hereby a drastic reduction of heat losses through the distribution of heat, a reduced use of fossil fuels in buildings and less dependence on energy prices can be achieved.



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## Modelling and Analysis of the Future European **Transmission System**

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The expected wide-spread deployment of intermittent renewable energy generation within the future European power system poses a range of challenges in the field of network planning and operation. The geographical distribution between renewable energy sources and areas of demand will require new transmission corridors that utilize both HVAC and HVDC technology, as well as upgrades of existing line capacities. Furthermore, in order to avoid overload of transmission lines during times of peak feed-in, new operational strategies such as the curtailment of renewable generation must be implemented. Additionally, the variability of renewable in-feed will require advanced conventional generator dispatch strategies in order to ensure sufficient generator ramping flexibility is provided.

As part of the 'Flexible Power Plants' project, potential solutions to these challenges are investigated through detailed modelling and simulation of the European transmission system. The requirements for line upgrades are investigated for various future development system scenarios and an optimal network planning algorithm is developed in order to identify the most suitable line upgrades. The adequacy of existing upgrade plans, such as the construction of HVDC links between north and south Germany, is assessed. The ability of renewable energy curtailment strategies to reduce the requirement for line upgrade is also investigated. Validation of proposed solutions is performed through AC load flow simulation of a high-resolution transmission system model. Finally, novel methods for unit commitment and dispatch of conventional generators are investigated, utilising detailed temperature modelling of power plants in order to allow for and adequate planning of flexibility resources in the system.



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### A Hybrid Transmission Grid Architecture For Improved Capacity Utilization

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Recently, Germany experiences a significant rise in electricity generation based on renewable energy sources, especially wind and solar energy, that leads to an increasingly distributed and fluctuating energy production. This requires the transmission grid to handle strong fluctuations and to smooth them via distribution, which ultimately asks for more transmission capacity. The effective transmission capacity depends on the physically installed capacity as well as the efficiency of its utilization. In our work, we propose a systematic upgrade of selected transmission lines that does not only increase the physical capacity but also supports the efficient utilization of the grid by offering a polynomial time solution to the optimal power flow problem. Furthermore, in simulations we show that this architecture also improves the power routing capabilities of the grid, enabling a more economic operation.

In the proposed upgrade process, all AC lines outside some arbitrary spanning tree of a given transmission grid are converted to high-voltage direct current (HVDC) lines as illustrated in Figure 1, leading to a hybrid transmission grid architecture. The conversion of AC lines to HVDC lines is a particularly appealing option to upgrade transmission line capacity, as HVDC lines feature a controllable power flow and provide dynamic voltage support at the terminals, which can further enhance the stability and transfer capability of the connected AC grid. In our work, we show that for this hybrid transmission grid architecture the operational task of determining an optimal utilization of the grid under given boundary conditions, i.e., the optimal power flow (OPF) problem, can be solved in polynomial time, which is in strong contrast to the NP-hard formulation for common AC transmission grids that lacks an efficient computational solution.

The transition to a hybrid transmission grid constitutes a significant investment in the grid infrastructure, even if transmission grids are typically sparsely meshed, i.e., the number of AC lines that are subject to an upgrade is small compared to the total number of AC lines. However, in the light of large shares of renewable energy sources for power generation, the effective power routing capability and efficient OPF solution method provided by the hybrid transmission grid may prove vital for congestion avoidance and the implementation of a frequent redispatch, allowing to maintain a stable operation and an adequate generation and demand balance.





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## Laser-ablated nanoparticles for hybrid photovoltaics

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Hybrid solar cells of inorganic and organic materials mark an important class of next generation solar cells, since they combine the advantages of inorganic materials, such as high stability, with the advantages of organic materials, such as tailoring of band gaps and potential low cost production.

We introduce laser-ablated nanoparticles into hybrid solar cells. The active layer consists of titanium dioxide nanoparticles produced by laser ablation in liquid and a water-soluble hole-conducting polymer poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T). The production of TiO<sub>2</sub> nanoparticles via laser ablation in liquid is achieved with two approaches, using a TiO<sub>2</sub> particle suspension as target and a solid titanium target [1]. The crystallinity of both components of the active layer, laser-ablated TiO<sub>2</sub> and P3P6T is investigated with X-ray diffraction (XRD) and grazing incidence wide angle X-ray scattering (GIWAXS). A key factor for the performance of the active layer is the functionalization of TiO<sub>2</sub> with the polymer P3P6T, which is probed with spectroscopic methods. The hybrid solar cells show high fill factors and open circuit voltages underlining the potential of the novel material and the environment-friendly processing method.



Figure 1: Laserablation in liquid for a suspension of titania particles, the illustration includes a 2D detector image of a GIWAXS investigation of functionalized particles, a sketch the built-up of the hybrid photovoltaic devices and an SEM image of laser-ablated particles

Based on the processing scheme we introduced [1], we develop an optimized setup for laser ablation in liquid. With metal wires as ablation target the target shape leads to less confinement of the plasma plume in the ablation process, also losses by heat dissipation are minimized in comparison to flat solid targets. With this we aim for a more efficient production of nanoparticles in a microfluidic sample environment.

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## **Residential Electricity Model**

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To develop strategies for improving the energy efficiency of cities it is important to understand the existing energy use patterns. This poster presents a novel approach for developing an accurate and realistic model of residential electricity demand using the city of Munich as a case study. It is part of a wider project "Energy Planning for Munich" undertaken by the Energy Efficient and Smart Cities group in exploring ways to make cities more energy efficient and carbon neutral.

A necessary property for the model is a flexible time and space resolution, to ensure its ability to evaluate different energy efficiency measures. The level of detail of the model is simulating the demand of single households with a time resolution of seconds. The model will take into account the randomness of human behavior by incorporating data about the variation of household sizes and lifestyles. Furthermore the aggregated demand of the total population should have the measured average load characteristics, i.e. those of the standard load profile. This approach uses both the standard load profile, and Activity Based Modelling using Time Use Surveys to simulate both single appliance loads.

Figure 1 shows the results of a simulation for a winter weekday for 1000 households. The Activity Based Modelling approach results in the red curve, whereas the scaled standard load profile is shown in green. This shows the importance of using the Standard Load Profile to determine the remaining loads, which should make up about 7% of the total energy consumption.



The model will be integrated with a spatial database which contains information of existing buildings in the metropolitan area of Munich, incorporating the distribution of household sizes in the various districts. This will allow realistic simulation of the household loads for the entire city. Once completed, the model can be used to evaluate various energy saving strategies and to test a wide range of policy and technology scenarios on building block or city quarter level.



## **HIPER – High Pressure Evaporation Rig**

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Conventional steam power plants often use water at super critical parameters as working fluid above the near critical pressure range (approximately located between 200 bars and 250 bars). Below the critical pressure of 221,2 bars the water may be thermodynamically at saturation state but the relatively small differences in density between liquid and steam let it behave similar to a supercritical fluid. At supercritical pressures water cannot undergo phase change when it is heated up. However, it shows significant steep changes of physical properties like an increased heat capacity by an magnitude of one thousand in a small temperature range [1]. This characteristic may influence both the heat transfer characteristics of the fluid causing rising wall temperatures and the flow stability leading to unpredicted behavior especially at subcritical pressures [2].

The current layout of state of the art power plants helps to avoid the use of fluids in the near critical region and limits the speed of transients at near critical states to ensure a safe operation of the plant. The present requirements of the energy transition may require a more frequent operation in this region by lowering the minimum load. Additionally it is required to realize faster load changes with faster changes of boundary conditions of the working fluid. Thus the questions of safe modes of operations with it's limits and useful strategies of control arise in order to adapt the existing power plants to the requirements of the actual energy transition. Furthermore, the present knowledgebase is predominantly based on steady state thermohydraulic experiments that have been conducted in the past decades.

To contribute to the energy transition a new test rig is actually under construction at the Institute for Energy Systems. The test rig HIPER (High Pressure Evaporation Rig) can operate up to 380 bars and reach temperatures of 580° C to cover the range of interest. By using throttle valves as actors a fast backpressure control is realized in combination with a speed controlled piston pump. This also allows to divide pressureand flow control by taking advantage of the steep performance curve of such pumps. The thermal inlet conditions of the experiments are controlled by an electrical preheater that is supplied with 700 kW, it can reach temperatures of up to 500° C. The evaporation experiments themselves are conducted in an instrumented tube that also is electrically heated with a maximum power of 300 kW. The geometric dimensions diameter and angle of the evaporator tube as well as the thermohydraulic parameters mass flux density and heat flux density can be chosen in a wide range that represents different layouts of actual and future power plants. The scientific dimensions that have to be measured mainly are wall- and fluidtemperatures, pressures, mass- and heat flux densities.

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## **Urban Energy System Modelling**

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Future urban energy systems will face the challenge to integrate distributed energy resources like photovoltaics and combined heat and power plants, but also storages and applications of electric mobility. A general architecture of domestic energy systems is described in Figure 1 and may contain a variety of generation, conversion, storage and load elements. In addition, the growing share of intermittent generation in today's energy system results in an increased demand for system flexibility on the consumer side.

Demand Side Management (DSM) strategies flexibilize the consumer demand by incentivising the reduction or shift of demand in time. In the context of integrated urban energy systems, coupling various energy sectors can offer benefits in the way of flexibility and better utilisation of resources and infrastructures. Power-to-Heat-solutions offer the possibility to use excess electricity generation from renewable sources for heating applications. Heat pumps in combination with hot water storages and the thermal mass of buildings can offer a certain DSM potential without affecting the residents' comfort (Figure 2).

The aim of this work is to develop a simulation framework to evaluate different DSM applications on the level of the local urban energy system. The benefits of optimizing urban energy systems on a building block or city guarter level rather than on an individual building level shall be investigated. This includes the quantification of impacts on the utilization and optimal sizing of electrical and thermal storages as well as a comparison of centralized versus distributed solutions and their control techniques. Among other features, the simulation framework requires modularity to master the range of different components within the system and scalability to enable the optimization for of a varying number of components.





### Development of a concept for energy optimization of existing Greek hotel buildings

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The current Master thesis investigates the energy performance of the hotel sector in Greece and proposes a concept for the energy optimization of existing hotel buildings on the basis of an exemplary project.

Hotel buildings are unique compared to other public, commercial buildings due to their varying size as well as their facilities and operating schedules. Recent studies indicate that hotels are the second highest energy consuming category after hospitals, while they are responsible for 10% of the total primary energy consumption and they reflect 28% of the total final energy use in the tertiary building sector of Greece, even though they represent only 0.82% of the building stock. According to the literature the reported average energy consumption for Greek hotels is 273kWh/m<sup>2</sup> annually.

Tourism is one of the main sectors of the Greek economy that motivates regional and national development and still offers employment opportunities. In 2012 the international arrivals reached over 15.5 million people leading Greece to the 17th place in the World Rankings, while in 2014 the total number is estimated to 21.5 million tourists.

As a case study, an existing hotel building, located in Thessaloniki, was selected in order to evaluate different energy optimization scenarios and calculate the potential energy savings. The Greek software TEE-KENAK, which is in accordance with the Directive 2002/91/EP of the European Parliament, was used for the energy simulations.

Based on three variants with different insulation standards - according to the existing building, the Greek TOTEE and the German EnEV - three main subjects were investigated: the building envelope, the electromechanical systems and the application of renewable energy technologies. The results of 72 different scenarios have been analyzed for each of the main Variants, leading to the final outcomes with an average reduction of 60% in the annual primary energy consumption.

These optimizations were also incorporated in the transformation of the main facade providing a new image for the hotel, while combining architectural and energy efficiency solutions. At the end feasibility parameters have been studied leading to the final results for the definition of a concept for the energy optimization of existing Greek hotel buildings.

This thesis makes consequently а contribution to understanding the energy use in hotel buildings and outlines the significantly high potentials for energy savings. It presents



that the targets set by Greece and the European Union on the energy efficiency of the building sector can be reached through refurbishment measures and architectural concepts, while hotels could function as pilot-demonstrators.

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Organic semiconducting materials can be applied in various optoelectronic devices such as organic lightemitting diodes and organic solar cells. The conductivity and optoelectronic properties strongly depend on the molecular morphology and crystallinity. Therefore controlling the thin film morphology is one of the main challenges when it comes to developing fabrication processes that work in small labs as well as in large industrial scales.

As many conjugated polymers are insoluble in most common solvents and do not allow a processing directly from solution, they are often further 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 an altering of the polymer's conductivity and optoelectronic properties.<sup>1</sup>

A promising approach to avoid changing the molecular structure of the conjugated polymers is synthesizing them in situ. For this purpose, the corresponding monomers are deposited onto the substrate and chemically linked afterwards. The monomers are usually soluble in many solvents and can easily be processed from solution. This procedure offers the possibility to obtain thin films of polymers without disturbing side chains.

In this work, active layers for organic solar cells are synthesized in situ and investigated regarding their morphology and optoelectronic performance. Derivatives of thiophene are employed as soluble monomers, deposited to the corresponding substrates and linked by an oxidative polymerization reaction.<sup>2</sup> The synthesized polythiophene (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.



Figure 1: Images of substrate (I) coated with adhesive layer, (II) with applied reaction mixture, (III) after polymerization reaction and (IV) after rinsing off reaction residues.

UV/Vis spectroscopy measurements of in situ PT films show a broad absorption in the visible range. Moreover, thermal post-treatment induces a formation of shoulders within the spectra, indicating an ordering of the polymer chains during the annealing procedure.

Grazing incidence wide angle x-ray scattering (GIWAXS) experiments are performed for investigation of polymer morphology and crystalline ordering of the polythiophene molecules.

Furthermore, the penetration of the applied fullerene layer into the polymer network with emphasis on the influence on the polymer packing are studied.

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### Electrocatalytic formic acid oxidation on supported Pt and Pd nanoparticles

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The electrochemical oxidation of formic acid (FAO) has attracted great attention because of its potential application in direct formic acid fuel cells (DFAFCs)<sup>1</sup>. Platinum and palladium are well-known catalysts in this reaction due to their high activity and stability. Despite extensive reports there are still many open

questions calling for further studies on these monometallic systems, especially, for understanding of the underlying effects from the catalyst itself and the environment. In this work, the activity and stability for FAO of Pt clusters supported on Au(111) as well as the size-dependent activity of Pd nanoparticles on highly oriented pyrolytic graphite (HOPG) are studied intensively.

Unselected  $Pt_n$  (n  $\ge$  35) clusters, which were generated in a laser-ablation cluster source with an average surface area of 0.92 nm<sup>2</sup> per cluster, were deposited on Au(111) by a soft-landing technique in an ultra-high vacuum (UHV) system<sup>2</sup>. This technique can produce uniformly dispersed and accurately size-controlled Pt clusters, which can simplify the study of the support effect of Au(111) to the Pt catalyzed FAO by varying the Pt surface coverage. Scanning tunneling microscopy (STM) indicates that the



clusters have an average height of around 1 nm. Figure 1 shows that the as-prepared Pt<sub>n</sub> clusters on Au(111) ( $Pt_n@Au(111)$ ) are more active than polycrystalline bulk Pt; additionally, the current density further increases with potential cycles. STM images measured on the same sample after 50 potential cycles do not show obvious particle agglomeration. The enhanced activity and stability of this Ptn@Au(111) can be attributed to the interactions of Pt<sub>n</sub> clusters as well as the support effect. With decreasing Pt coverage, the potential of the major oxidation peak shifts to a higher value, which indicates that the Au substrate weakens the adsorption energy of Pt<sub>n</sub> clusters to the formate ions.





Figure 2: (A) Linear sweep voltammetry of bulk Pd and Pd/HOPG samples in 0.5M H<sub>2</sub>SO<sub>4</sub> + 0.5 M HCOOH at a scan rate of 20mVs<sup>-1</sup>. (B) The specific current density for FAO at 0.4V vs. RHE. Bulk Pd was used as a reference.

the specific current density for FAO at 0.4V vs. RHE. The peak potentials of the small particles are more negative than those of the bulk Pd and larger Pd particles, which can be attributed to the formation of a poisoning intermediate on the smaller particles at a lower potential. The results suggest that the smaller Pd nanoparticles are less active than larger ones due to the strong binding between Pd atoms and reaction intermediates.

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### **Global Dynamic Sensitivity Analysis of Transient Simulations of Residential Quarters**

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In the future, renewable decentralized energy supply of buildings will become more and more important and due to the fluctuation of the renewable energy sources the focus of energy demand and supply calculations will switch from the cumulative monthly or annual energy demand to a detailed hourly examination, for both electric and heating systems. The existing buildings offer a huge range of possible refurbishment measures and the effects of these measures have to be considered in a detailed examination in order to select the best option regarding all relevant target functions like overall energy demand, necessary peak power, thermal comfort or self-sufficiency for electricity.

In this paper an approach for using global dynamic sensitivity analysis to assess the effects of different building refurbishment measures will be presented. The methodology is part of the author's dissertation.

The method of elementary effects (Morris 1991) modified in (Campolongi et al. 2007) can be used to calculate sensitivity measures in an efficient way. In the first approach, the sequential sensitivity analysis, for every hour of the year and for every parameter an independent sensitivity measure is calculated. In a second approach, a principal component analysis will be used to get a dimensional reduction of the results. The sensitivity measures are calculated for the representation in the principal components, the challenge here is to describe the meaning of the principal components in dependence of the simulation results. A third approach uses a technique called 'impulse parametric sensitivity analysis' (Perumal, Gunawan 2011), which is already established in computational systems biology. With this method the influence of impulse inputs like the switch-on of a heating system and especially the importance of the time of switch-on can be assessed. The method has to be modified to be usable in connection with the elementary effects method.

The methods described above will be used to identify the sensitivities of the parameters of a simulation model, which uses building typology data, GIS data and additional statistical information to parametrize independently running transient EnergyPlus models.

A future step will be to include the coupling of the EnergyPlus simulation models using the Functional Mockup Interface to be able to calculate effects arising from demand side management measures like increase of set point temperature in times of high electrical energy production from renewables or switch-on of additional household applications. This will enable the model to simulate the interactions in a city quarter.

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### Low band gap polymers – the future in organic photovoltaics?

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Among the next generation solar cells, in particular organic photovoltaics are gaining impact as a feasible alternative to conventional silicon solar cells. Using polymer films as active material for the energy conversion has several potential advantages, for instance the material availability and low-cost processing techniques. Due to the potential device flexibility and tunable colors and shapes, organic photovoltaics could be integrated into a wide range of applications, combining functionality with design in fields as diverse as mobility, architecture or clothing. However, efficiencies of polymer solar cells stay far below those of commercially available inorganic photovoltaics.



images of various compositions of PTB7-Th:ICBA

In order to enhance the solar cell performance, recent research efforts focus on identifying new, highly efficient polymers. This has led to the development of low band gap materials with reported solar cell efficiencies approaching 10 %. Our work focuses on a group of high-efficiency polymers called PBDTTTs. Due to their low band-gap they show an overall increase in the absorption of light. Functional groups can be introduced in order to increase the efficiency even further. A high degree of fluorination shows favorable effects on the solar cell performance, as has been shown for the prominent example PTB7. Exchanging oxygen with thiophene units in PTB7 leads to a

new polymer called PTB7-Th with an even further reduced band gap. Reported record efficiencies for PTB7-Th based solar cells recently broke the important barrier of 10 %.

Previous morphological investigations linked to the device performance give first insights into the working mechanisms of PBDTTTs. We concentrate on investigating the optical and morphological properties of model systems using PTB7 and PTB7-Th. Applied characterization techniques include optical absorption measurements, optical and atomic force microscopy, X-ray reflectometry and diffraction as well as advanced scattering methods such as grazing incidence small and wide angle X-ray scattering. Exploratory solar cells link the power conversion efficiency to parameters such as the active layer composition and morphology.



Figure 2: Wavelength-dependent absorption of thin films with various compositions

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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.  $MN_xC_v$  system (M = Fe, Co) are favored due

to their low cost, reasonable activity and remarkable

selectivity towards ORR<sup>1</sup>. On the other hand, MN<sub>x</sub>C<sub>y</sub>

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<sup>2</sup>, 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 systems, starting with

### ZrO<sub>2</sub>/C as Noble Metal-free **Oxygen Reduction Reaction Catalyst in 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.



Figure 1: X-ray diffractograms of carbon supported zirconia nanoparticles synthesized from two different precursors

phthalocyanine (ZrOPc) and zirconium acetylacetonate (Zr(acac)<sub>4</sub>). The difference in atomic constitution and solubility in dispersing medium of the two precursors made their use and the investigation of the obtained interesting. Figure 1 catalyst shows the X-ray diffractograms of supported zirconia nanoparticles from both the precursors. To the samples synthesized from ZrOPc at ≥900 °C and from Zr(acac)<sub>4</sub> at ≥750 °C a t-ZrO<sub>2</sub> phase assignable. Furthermore, the is ORR electrochemical activity of these samples was tested by thin-film RDE technique at 20 °C in 0.1 M HClO<sub>4</sub> electrolyte (Figure 2)<sup>4</sup>. Comparing the ORR results, it is clearly seen that, in the synthesis-temperature range of 750-1000 °C, ZrO<sub>2</sub>/KB from ZrOPc shows an appreciable activity while the supported zirconia from Zr(acac)<sub>4</sub> has a negligible activity. From the structure of the precursors we infer that the nitrogen from ZrOPc acts as doping agent and/or creates oxygen vacancies in ZrO<sub>2</sub> structure, providing in this way some ORR activity. To support our hypothesis



Figure 2: Difference in ORR activities of synthesized zirconia nanoparticles

and to further increase the ORR activity we would like to synthesize and characterize 'doped zirconia' with metal dopants like yttrium (reported to create oxygen vacancies in ZrO<sub>2</sub> structure), nitrogen etc<sup>5</sup>. Structural and electrochemical characterizations will be performed as before.

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## **Relating Process Parameters** to Energy Consumption

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Environmental management and energy management play an ever-increasing role for a large number of small and medium-sized enterprises (SME). This is due to two facts. Firstly, energy costs are continuously increasing, which has a negative impact on the profit of producing companies, e.g. in the paper industry the share of energy costs in relation to the gross output value amounted to seven percent in 2012 [Sta14]. Secondly, legal regulations, such as the law for the development of renewable energies [Eeg14] and the DIN EN ISO 50001 [DIN11], pose new challenges for SMEs, e.g. by requiring companies to establish a dedicated energy policy and management.

In order to allow acquisition and summarization of the energy consumption of a company, DIN EN ISO 50001 requires companies to define energy performance indicators (EnPI). For some parts of a company, e.g. those that solely rely on electrical energy, the definition of EnPIs is a straightforward approach. On the production level however, this is much more difficult. One of these difficulties is the lack of transparency between process parameters and the energy consumption of the plant. To approach this problem, it is essential to not only have knowledge about the influence of each parameter concerning the production process, but also about how each parameter affects the energy consumption.

Therefore, the goal of the project ProMES is to develop a novel approach to identify and analyze prominent as well as hidden relations between process parameters concerning energy consumption within a production plant with the goal of identifying possible energy saving and optimization potentials. For this purpose, plants and their process values plants are analyzed in order to uncover existing parameter dependencies. To allow continuous optimization, the identified dependencies have to be compared to live process data. Hence, the dependencies are modelled using an extension of the MES-ML, a language to model technical systems, their processes and data flows. In order to enable extensions to the existing MES-ML standard, the modelling is performed, using a graphical editor, developed by the Institute of Automation and Information Systems. Based on these dependency models, EnPIs are constructed and real-time recommendations to reduce the plant's energy consumption can be provided to the plant's operator.

According to the industry partners consulted during the project's initial phase, personnel with different educational backgrounds, e.g. technical personnel, operators or management, have to be able to use the analysis tools. Therefore, insights into the plant's energy consumption need to be displayed hierarchically, which allows for different views of the plant.

In order to allow specification of energy losses due to waste incurring during production, the energy content of the product produced also has to be taken into. Consequently, to establish a comprehensive overview of the overall energy efficiency of a plant, the process as well as the product have to be modeled.

The presented work provides an overview over the motivation, goals and progress of the project and offers insights into best practices when identifying energy flows within production plants.



### **Block copolymer based membranes** for lithium ion micro 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: Skematic illustration of lithium salt incorporation in PS-b-PEO diblock copolymer In this work, the morphology of lithium ion-polymer hybrid material [1] based on high-molecular-weight polystyrene-blockpolyethylene oxide PS-b-PEO diblock copolymers at different temperatures and salt concentrations is investigated. The use of block copolymers enables the formation of conductive lithium containing polyethylene oxide (PEO) domains as well as mechanically stable glassy polystyrene (PS) domains. The tendency of the PEO block to crystallize is highly suppressed with increasing both, the salt doping level and the temperature. As indicated from small-angle X-ray scattering (SAXS) measurements. the PEO chains change from а compact/highly folded conformation to an

amorphous/expanded-like conformation upon salt upload. Additionally lithium containing polymer samples are sandwiched between two metal electrodes and the film conductivity is measured using impedance spectroscopy. The effects of both temperature and the salt concentration on the ionic conductivity are demonstrated [2].

An enhanced ionic conductivity is found to be correlated to the enhanced microphase separation of the lithium containing polymer. The ionic conductivity is enhanced by the PEO amorphorization and thereby the mobility of the PEO blocks increases upon increasing the salt doping level. 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.

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## Morphology of Polymer-Metal Interfaces

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Within recent years, metalized polymer films have attracted great interest due to their applications in organic field effect transistors (OFETs), organic light emitting diodes (OLEDs) and organic solar cells (OSCs). In these devices, a thin metal layer is used as an electric contact in conjunction with an active layer comprising a semiconducting polymer. Thereby, charges can either be injected into the active layer or extracted from it. The charge injection or extraction is strongly influenced by the electronic properties at the interface of the metal/polymer film. In order to obtain the desired electronic properties, a precise control of the metal growth on top of the polymer is required.



Figure 1: Working principle of GISAXS. The image was taken from reference [1].

The metal growth on top of the polymer can be studied by in-situ grazing incidence small angle x-ray scattering (GISAXS) experiments. GISAXS (see Fig. 1) is a versatile and non-destructive tool to obtain averaged and statistical information on structural shapes and sizes on a nanometer scale. In addition, GISAXS allows studying structures which are buried below the surface of a material and which are therefore inaccessible to conventional imaging techniques such as atomic force microscopy (AFM). When combining GISAXS with a dedicated ultrahigh vacuum (UHV) setup for vapor deposition processes, in-situ GISAXS experiments can be performed. In-situ experiments offer the possibility to monitor the growth process in real-time yielding important information on the growth kinetics. Thereby, one is able to extract temporal information on structural

parameters such as cluster size, shape and spatial distribution. Using these parameters, a model for growth control can be derived. Recently performed time-resolved GISAXS measurements showed that

different growth models apply for the metal/polymer systems gold/poly(N-vinylcarbazole) (PVK) and aluminum/poly(3-hexylthiophene) (P3HT). While gold grows in 3D clusters on PVK, aluminum follows a layer-by-layer growth model on P3HT (see Fig. 2). The layer-by-layer growth is favorable since a large contact area is achieved which allows a high charge transfer across the metal/polymer interface reducing the contact resistance. In addition, a large contact area leads to good film adhesion and avoids the

delamination of the metal film.

In the presented work, we extend the studies of the aluminum/P3HT system. In-situ GISAXS measurements are performed to investigate

aluminum on P3HT for different molecular



the growth kinetics of Figure 2: In-situ GISAXS study of an aluminum sputter deposition process on P3HT. The images were recorded after 0, 5, 10, 15, 20, 25 and 30 min. The image was taken from reference [2].

weights of the polymer. The study is complemented by different imaging, optical and electronic characterization methods.

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### Preparation and characterization of microporous layers for PEM fuel cell diffusion media

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Polymer electrolyte membrane fuel cells (PEMFC) are electrochemical devices, which use the reaction of hydrogen and oxygen to produce electrical energy. On the anode hydrogen is oxidized giving protons and electrons and on the cathode oxygen gets reduced to water consuming electrons and protons. The anode and the cathode are separated by a proton conducting membrane forming the so-called membrane electrode assembly (MEA).

The gas diffusion layer (GDL) is an important component of PEMFCs. It is sandwiched between the MEA and the gas flow field on both anode and cathode. Usually it consists of a hydrophobic treated carbon fiber substrate and of a thin microporous layer (MPL) of carbon black and a PTFE-binder. The main requirements for GDLs are mechanical support, electrical and thermal conductivity, reactant gas distribution and water management [1]. The MPL, which is facing towards the electrodes, has various functions: (1) reducing thermal and electrical contact resistances, (2) mechanical protection of the membrane and (3) improving the liquid water transport. Particularly for automotive application, where a high volumetric power density is required, fuel cells are operated at high current densities and therefor produce a lot of water, which condenses in the electrodes and GDLs. Hence, the transport of reactant gas to the electrode is hindered by a reduced effective porosity [2].

The goal of this work is to prepare different model MPLs to investigate the influence of various MPL properties on the water management in PEMFCs. To fabricate microporous layers we prepare aqueous inks containing carbon black, polymer binder and additives. The inks are grinded on a roller mill in order to disperse the carbon. After that the inks are coated on a commercial carbon fiber substrate and are subjected to a heat treatment. The dispersions are investigated by rheometric measurements. To characterize the coatings scanning electron microscope (SEM) is used and the four-point through plane resistance is measured. In fuel cell tests the GDLs are benchmarked with commercial materials by recording polarization curves at various dry and wet operating conditions.

In our study we will illustrate a viable method to prepare MPLs with a homogeneous surface structure and will show how the preparation technique influences the layer properties. On that basis we plan to vary MPL properties, such as porosity and hydrophobicity to investigate their influence on transport phenomena in a fuel cell.

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## The morphology of perovskite solar cells

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Increasing worldwide demand for cheap energy and the problem of climate change necessitate the use of carbon emission free sustainable energy sources for future energy production. The most abundant and widely available source for such renewable energy is solar power. The two biggest problems for implementing solar energy as a major energy source are the high panel and installment costs on the one side and the problem of storing the harvested energy on the other side. The first one could be addressed through new solar cell materials and the second one through better battery technology.



In recent years lead halide perovskites have attracted increasing attention as a new solar cell material due to a rapid increase in the power conversion efficiency (PCE) from 3.9% in 2009 to 20.1% in 2015 for solar cells fabricated with methylammonium lead iodide (MAPbl<sub>3</sub>) as the active layer. The latter is already comparable to established thin film solar cell technologies or to the silicon solar cells typically used in commercial applications today. The abundancy of the elements used in these cells combined with the possibility of processing lead halide perovskites in solution might allow for much simpler and cheaper production of solar cells based on these materials through techniques such as roll-to-roll processing or spraying.

Reasons for the good performance of lead halide perovskites in solar cells are favorable material properties such as strong absorption, large charge diffusion lengths, and benign defect physics.

Figure 1: The structure of MAPbl<sub>3</sub>

Despite the quick increase in PCE the relationship between preparation method, film morphology and solar cell performance is still poorly understood.

We aim to understand this relationship by investigating the link between the crystal structure (see Figure 1) of the material, the orientation distribution and size of crystallites within the film (see Figure 2 for the 2D detector picture of an X-ray scattering experiment, which allows us to measure the orientation distribution within the film) and the photovoltaic performance of the resulting devices for a variety of different fabrication methods in order to find guidelines for rationally designing methods for better performance.



Figure 2: GIWAXS detector picture of thin perovskite film

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## **Transparent Plastic Electrodes: Printing from** polymeric solution and following crystallization in-situ

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Organic electronics (OE) and organic conducting thin films have attracted much attention in recent years. For a better understanding of the complex behavior of these materials, there have been numerous studies to couple the electronic performance with the morphology.

Laboratory-based methods, such as spin coating, solution casting, doctor blading or dip coating, are extensively used for the preparation of thin film OEs and for subsequent characterization. However, one of the strongest motivations for OEs lies in the potential of fabricating flexible devices that can be scaled-up for industrial processing where laboratory-based processes do not apply. Large scale coating processes, like spray coating, rotary screen printing, flexographic printing, or slot die coating are the industrial standards for printing OEs. Slot die coating, in particular, is a very cost-effective production technique that offers the possibility of large scale manufacturing and custom-designed pattern coating.

The strongest advantages of organic electronics over classical semiconductors are the possibility of fully flexible devices and easy up-scaling, e.g. by slot-die printing. For fully printed and flexible devices there is a strong need for non-brittle and solvent processed electrodes, such as highly conductive poly(3,4ethylenedioxythiophene):poly(styrene-sulfonate) (PEDOT:PSS), a polymer mixture which are in general also called plastics.



Film properties are strongly correlated to the films nanomorphology and with this strongly depend on the processing technique used. We investigate the film evolution and crystallization of highly conductive PEDOT:PSS transparent electrodes in-situ during the printing process.

We thereby monitor the film evolution by in-situ grazing incident wide angle x-ray scattering (GIWAXS). Five film formation processes are detected, the crystallization of the polymers is correlated to solvent evaporation and enhanced interchain coupling is induced by the use of high boiling point co-solvents as ethylene glycol. The conductivity enhancement by more than three orders of magnitude in co-solvent treated PEDOT:PSS films is related to enhanced interchain coupling, crystallite sizes and molecular orientation.

Additionally, understanding the film evolution during the printing process could allow for tailored modifications of the solutions and printed films thereby gaining further enhanced OE device performance. By controlling the  $\pi$ - $\pi$  stacking distance of PEDOT with the amount of EG in the system the conductivity of PEDOT: PSS films could be controlled.

Reference: C. M. Palumbiny, F. Liu, T. P. Russell, A. Hexemer, C. Wang, and P. Müller-Buschbaum, Advanced Materials 2015, accepted

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### An insight into Li-ion battery research using X-ray and neutron scattering techniques

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Lithium-ion batteries are widely used in portable electronics and are considered as ideal candidates for hybrid vehicles as well as for stationary storage systems. There is a continuous search for new anode materials with higher energy and power densities. Morphology of the electrode plays an important role in balancing the two criteria because lithium diffusion rate (which influences the power density of a battery) is proportional to the square of the electrode thickness (which influences the energy density of a battery). We will show how statistically averaged size distributions and porosities of nanostructured electrodes can be effectively determined using grazing incidence small- angle x-ray and neutron scattering techniques.<sup>1</sup> These parameters are important to interpret the electrochemical performances of these new anode materials in batteries. Moreover, we will show how in situ diffraction techniques in transmission mode can assist in determining possible reasons for capacity fade after long-term cycling of LiFePO<sub>4</sub> – graphite cells. The advantage of neutrons over X-rays in diffraction studies of Li- ion batteries will also be highlighted.

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### Wind farm cooperative control: methods and experimental verification

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In the past, most of the research in wind energy technology focused on the optimization of wind turbines. In recent years, interest has expanded from the level of the individual machines to the one of wind farms. Optimal site selection, layout and control of wind farms are extremely challenging tasks that require an understanding of the aerodynamic interactions among the various machines and with the environment. These are all problems that are not yet fully understood and that are still challenging to model in an accurate way.



#### Figure 1: at left, wake and turbulence effects in a wind farm; at right: power curtailment and wake deflection strategies for wind farm cooperative control.

In this contribution, we describe our ongoing work on wind farm control. Ad hoc observers are used for detecting wake interaction conditions, in turn enabling cooperative control strategies for power maximization and load mitigation by power curtailment and active wake deflection. Our research program includes a scaled experimental facility for the simulation of wind farms in a boundary layer wind tunnel, which is used for the validation of simulation tools and the verification of control strategies.



Figure 2: at left, scaled wind turbine models; at right: experimental setup in the wind tunnel for the testing of wind farm control strategies.

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# Manufacturing of LFP electrodes: From laboratory to large-scale production

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Lithium iron phosphate (LFP) is an inexpensive cathode material for lithium-ion batteries with superior electrochemical properties. Due to the cycling stability over 10.000's of cycles and low safety risks, this material is ideal for stationary energy storage. Lithium iron phosphate has a theoretical specific capacity of 170 mAh/g at an equilibrium potential of 3.5 V vs. Li/Li<sup>+</sup>.

Producing energy out of solar power and wind energy is getting more and more common, but without storage the power supply system is destabilized and the energy produced out of renewable resources cannot be used. Therefore stationary energy storage systems are needed. In the EEBatt project the TUM and partners from industry are working together to build a stationary energy storage system, the so called ENERGY NEIGHBOUR, which has a capacity of 200 kWh, funded by the Bavarian Ministry of Economic Affairs and Media, Energy and Technology.

The aim of this work is the scale-up of LFP-inks for the production of 5 Ah LFP/Graphite pouch cells at the iwb (Institut für Wergzeugmaschinen und Betriebswissenschaften, TUM). In order to translate parameters from the laboratory into large-scale production numerous experiments have to be carried out.

First of all, LFP-electrodes are produced and tested in small laboratory test cells, to find the optimum composition of the electrodes concerning electrochemistry. This is achieved by application of different (electrochemical) techniques such as galvanostatic cycling, impedance spectroscopy as well as scanning electron microscopy (SEM). In figure 1 a SEM image of a self-prepared LFP electrode is shown. Figure 2 shows a typical rate-test, performed with LFP-electrodes.

As the electrode ink consists of the active material LFP, a binder, conductive carbon and the solvent NMP, the rheological properties of these inks, which are important for large-scale production, are investigated and optimized towards a high solid content at low viscosity. The properties and their dependence on the composition of the inks are studied with a rheometer and a particle size distribution analyzer. A further aim of this work is to understand how parameters like viscosity and solid content of the inks affect the coating process.





Figure 1: SEM cross-section of a LFP electrode Figure 2: Discharge rate test of LFP-electrodes with different loadings carried out in half cells after cccv cross-section with a loading of 55.46 mg/cm<sup>2</sup> at a magnification of 5000. charge.

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## Following the evolution of nanostructure in active layers of printed 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 an enormous drawback in terms of environmentally friendly processing of inorganic devices. Organic



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

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. A large variety of printing and coating techniques are used to reach this goal, among others knife coating, slot-die coating, screen printing or spray coating. During development, however, a lot of effort has to be spend 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 is a challenge and a better

knowledge of the structure 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 yet about the appropriate development in printed systems.

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 its assembly due to different electron densities. The scattered intensities are recorded on a 2D-detector and map the so-called reciprocal space. Via Fourier transformation, real space information are obtained. 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). We obtain an insight



solar cells exhibit among others, the advantage of high absorptive materials reducing the needed amount of materials. Furthermore, a key advantage of organic photoactive layers is the possibility to be

processed 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 upscaling to industrial-oriented scales which

Figure 2: Model of structure formation

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.

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### Phase separation and crystallinity in nanocomposite **PS-PEO** copolymer electrolytes

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Novel portable electronics, electrical and hybrid cars, and medical devices demand for environmentally friendly, health-safe, and economical energy storage devices with fast charge rates, high power density and outstanding capacity [1]. Lithium cations (Li<sup>+</sup>) provide an exceptional charge to mass ratio. Thus, a lot of attention is paid to secondary batteries with Li<sup>+</sup> as charge carriers. An effective electrolyte for such devices should facilitate mobility of Li<sup>+</sup>, restrict mobility of electrons, provide mechanical integrity, remain chemically stable up to high temperatures, and retain its properties over charge-discharge and heating-cooling cycles.

Polyethylene oxide (PEO) is commonly utilized as a dry polymer electrolyte, however it has two significant drawbacks: at operational temperatures it shows poor mechanical stability and its crystallites tend to inhibit ion mobility. Copolymerization with a glassy component has been proposed as a solution to the poor mechanical properties. Further, incorporation of nanoparticles is expected to provide additional mechanical strength while suppressing crystallinity. Such a system, ideally, should be highly phase separated in glassy domains providing mechanical integrity and fully amorphous, rather wide domains, which will serve as cation pathways.

We solution blended SiO<sub>2</sub> nanoparticles (12 nm) into an electrolyte system which consists of a PS-PEO diblock copolymer as matrix, and bis-trifluoromethane sulfonamide lithium salt (LiTFSI). In this initial stage

of our research, we study the crystallization properties and phase separation of the system by Differential Scanning Calorimetry (DSC) and X-ray scattering in a broad g-range 0.03 – 20 nm<sup>-1</sup>.

Both techniques reveal that a LiTFSI doping of Li<sup>+</sup>:EO = 0.1 molar ratio already eliminates crystallinity [2]. The matrix copolymer is organized in lamellae. This structure is retained upon addition of the salt, but the lamellae are considerably thicker. Insignificant variations of the thickness of the lamellae are caused on addition of nanoparticles. However, we may observe that the SAXS peaks (Figure 1) become significantly thinner at 1 wt% loading, possibly indicating that the lamellae are more extended. The structure remains unaffected over a temperature range of 30 to 130 °C.

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#### "Room-only" analysis for building energy assessments

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The identification of energy saving potentials needs reliable assessment methods. In practice assessment methods are either data driven or based on measured data. Normally simple building assessment methods are easy-to-use, but limited in their amount of information and model flexibility - the opposite holds for complex methods.

The complexity of heterogeneous buildings increases this conflict. As an example, universities are heterogeneous according to diverse construction types, designs, HVAC-systems, building use and occupant behavior. Complex buildings need more comprehensive assessment methods to fully consider their individual characteristics. Every theoretical model is based on simplification and due to this fact, uncertainty about the results is introduced by input parameters and model assumptions. The effect of uncertainty has to be taken into account even though there are huge efforts for the estimation or constraints to the model complexity. Both complex models and the implementation of Monte Carlo simulation techniques leads to long runtimes to achieve the desired results, especially for uncertainty and sensitivity measures.

The Reference room-Method (RRM) is a simplified approach of a whole-building simulation, which decreases runtime significantly and offers the opportunity for the implementation of time expensive statistical methods. The RRM could be described by using typical rooms only for energy and thermal behavior calculations, followed by the accumulation of each energy result considering specific floor space demands. The well-known and validated EnergyPlus engine is used as calculation core.

The following results are based on a first comparison of a Monte Carlo simulation of a homogeneous office reference building model (BM) with a one-zone model for a single room (ZM) with a sample size of 250. The analysis resulted in mean heating energy demand  $\mu_{BM}$  = 54.8 kWh/m<sup>2</sup> and  $\mu_{ZM}$  = 45.7 kWh/m<sup>2</sup>, the standard deviation  $\sigma_{BM}$  = 22.7 kWh/m<sup>2</sup> and  $\sigma_{ZM}$  = 22.3 kWh/m<sup>2</sup>. A significant difference between the mean values was found using the t-Test as shown in Table 1. A reliable estimation of the real mean value is to be unlikely without an appropriate adjustment. The statistical tests for equality of variance do not reject the null hypothesis meaning equal variances are assumed for both models. The future implementation of variance based sensitivity techniques seems promising to identify main impact factors based on "first-order indices" and "total-effect indices" even with simplified models.

One first qualitative sensitivity measure is the standardized regression coefficient (β-value). The regression coefficients are normalized according to input parameter-variance to result-variance. Values are between 0 (no impact) and 1 (highest impact). Only qualitative rankings are possible, e.g., Input\_1 is more important than Input\_2. Figure 1 shows a similar fit of the  $\beta$ -value for BM and ZM for 12 different basic setups. Both models indicate that the Uvalue of windows is the most important factor for heating energy demand, followed by infiltration rate and SHGC of windows.

The RRM is still under research and development for heterogeneous buildings. The presented results are promising for a quick and reliable assessment of heterogeneous buildings after the specified constraints are solved.



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## **OpenGridMap: Crowdsourcing Power Grid Data**

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In order to achieve the goals set by the energy reform of 2014, the current German power grid needs to be modernized and expanded. One of the main challenges for researchers and industry experts is the access to realistic power grid data. We believe that the access to more accurate and realistic data will lead to more efficient solutions that can be tailored to address specific issues on the current power grid. With this in mind, we launched the project OpenGridMap. The goal of the project is to develop a platform for the collection, visualization and management of power grid data to offer a realistic estimation of the current power arid.

A recent survey in the US revealed that 23% of the electric distribution utility companies have incomplete data of their networks and over 30% have outdated data. In Germany, over 90% of the renewable energy installed capacity is connected at the distribution level and with a length of over 1.7 Mio km, the electric distribution network makes over 98% of the entire power grid. Sadly, although the distribution network plays such an important role, its data is the hardest to come by for researchers. Often, this data is not public, is unknown, or is outdated and ultimately wrong. This forces researchers to work with test grids, which represent only the average and do not accurately represent the reality of many power grids. One solution to this problem is to collect data of realistic power distribution networks. However, traditional collection of this data is difficult, expensive and intrusive. To overcome this, OpenGridMap proposes the use of crowdsourcing for data collection. Crowdsourcing has been proven to be a reliable and affordable method for data collection in other areas, but its use in the power system context remains yet to be studied. The workflow that OpenGridMap uses in order to obtain realistic power grid data can be seen in the figure bellow.

Collection: OpenGridMap uses available geographical data as well as data collected through our own smartphone app. The app allows the collection of several pictures and GPS coordinates of power grid elements. Different elements can be collected through the app and pushed to a server for storage and management. Currently, our app is called grid2osm and can be found on Google Play.

Verification: The data collected by the smartphone app has to be verified and classified. For verification, we propose the use of machine learning algorithms to verify that the mapped elements are in fact power grid elements. Once an element has been verified as a power grid element, it is stored on a database and can be visualized for classification. Currently, we solve the task of classification by having experts in the loop that can classify specifically what kind of power grid element was mapped.

Inference: After collecting enough power gird elements we can infer the structure of the power grid. Since we know where important power grid elements like substations, transformers, loads and generators are, we can offer a realistic estimation of how the actual power grid probably is.

Analysis: Finally the inferred power grid will be made available to other applications for classical power system analysis.

Within the workflow described, we plan to have several feedback loops, e.g., between analysis and inference, and also between analysis and collection.

Ultimately, OpenGridMap can become a complementary tool for the collection of power grid geographical data and offer an affordable power geographical information system to utilities, researchers and industry experts all over the world.

The OpenGridMap project started in March 2015 and has a duration of 2 years. The app and platform are currently on alpha testing and it URLs can be found bellow. OpenGridMap is an open source project and all its code can be seen in github.com/opengridmap. We are actively looking for partners and contributors.

Collection Verification Analysis Inference CSV EnergyMap.info GridLAB-D

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### Degradation in organic solar cells: Why structure matters

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Based on their physical principles, organic solar cells (OSCs) open fields of application that are not accessible by conventional silicon-based photovoltaics. OSCs based on a thin blend film of a semiconducting polymer and a fullerene derivative thereby can be produced via a fully wet chemical route which paves the way towards cost-efficient large-scale production even on flexible substrates by roll-to-roll printing or spray deposition. Their mechanical flexibility, their optional optical transparency ant their potentially low fabrication cost render organic solar cells suitable for a large field of applications ranging from use as current-generating windows in architecture to mobile power sources in barely tapped regions.



Figure 1: OSC stack (left) and morphological

degradation (right).

However, challenge to face is given by the faster device degradation as compared to silicon-based photovoltaics. One major reason for degradation is hereby caused by structural changes of the active layer of the solar cell: Light that is absorbed by the polymer in the active layer creates a localized excited state which can travel on a short length scale but it can be split into free charge carriers only if it meets an interface between polymer and fullerene domains within this distance (see Figure 1, left). A change of active layer morphology (depicted in Figure 1, right) drastically changes the probability of charge carrier separation and therefore can lead to device

degradation. Our group has recently presented a first evidence for this pathway of degradation by simultaneously monitoring both the coarsening active layer morphology and the deteriorating performance of an operating solar cell based on poly-(3-hexyl-thiophene) and C<sub>60</sub> butyric acid methyl ester (P3HT:PCBM).<sup>[1]</sup> A next step towards a full understanding of morphological degradation is now due by investigating the exact mechanism for different systems, especially when solvent additives are used during fabrication. However, the initial morphology and the impact of solvent additives need to be completely clarified as a prerequisite.

In the presented work we illuminate the nanometer and sub nanometer scaled morphology of thin blend films from the low-bandgap polymer PCPDTBT and C<sub>70</sub> based PC<sub>70</sub>BM. It is known that, hereby, the use of small amounts of 1,8-octanedithiol (ODT) as a processing additive improves solar cell performance drastically.<sup>[2]</sup> We investigate the impact of both, blend composition and ODT, on the nanometer and sub-nanometer scale morphology by using Grazing Incidence Small and Wide Angle Xray Scattering (Figure 2) and X-ray reflectivity measurements. The data is complemented by optical absorption spectroscopy in the UV and visible range. It is found that ODT leads to both enhanced micro phase separation Figure 2: Schematic GISAXS setup and polymer crystallization and eliminates the dependence on blend



composition in a large range. Furthermore, ODT is found to expulse fullerene from the blend layer. All findings give reason to enhanced photovoltaic performance.

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### Non-ideal torque control in wind turbine systems: **Causes and impacts**

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Power generation with wind turbines is onshore already today a competitive alternative to fossil power generation with respect to the levelized costs of energy. The biggest part of the costs for wind power are the investment costs. So the cost per kWh mostly depends on the "produced" amount of energy.

One reason for reduced energy production is non-ideal torgue control: The generated torgue does not equal the demanded torque. This is possible because state of the art wind turbines are not equipped with a torque sensor and so there is no feedback for torque.



Figure 1: Simplified structure of a wind turbine control-system with possible causes for non-ideal torque control.

Causes for non-ideal torque control are faults or deviations of sensors (see 4 in Fig. 1) or in signal communication (see 4 in Fig. 1). Further causes are deviating system parameters (see 4 in Fig. 1) from values used for controller design or unknown friction losses in the drive train. All these effects result in a deviation of the generated electrical torque from the torque required for maximal energy production of the wind turbine.

The impact of a non-ideal torque control is calculated for a variable-speed pitch-controlled wind turbine. The calculations are conducted based on real wind data. The poster shows the reduction of the total energy production as well as the lost earnings for the different operation modes (e.g. partial load and rated power).

The results point out, that non-ideal torque control can cause a significant reduction of the produced power in wind turbines. Therefore this issue should be investigated more thoroughly and solutions have to be found.



### Investigating the morphology of MAPbl<sub>3-x</sub>Cl<sub>x</sub> highly efficient perovskite solar cells

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In the past years, organic-inorganic hybrid materials with perovskite crystal structure have received much attention as promising absorber materials for future photovoltaics. Perovskite solar cells not only offer the opportunity of easy and potentially cheap processing techniques comparable to organic and dyesensitized solar cells - gradual optimization of preparation routines has led to power conversion efficiencies (PCE) of over 15 % for solution processed devices, thus challenging conventional thin film technologies like microcrystalline silicon, CdTe and CIGS solar cells. These high power conversion efficiencies can be traced back to the remarkable properties of the highly-crystalline perovskite absorber like high intrinsic absorption, exceptionally high open circuit voltages exceeding 1 V and ambipolar electron and hole transport with large diffusion lengths, which allows for a planar cell design. However, fundamental understanding of some basic working principles lacks behind the fast progress in device efficiency. The most challenging questions tackled by scientist are



Figure 1: Distribution of crystal sizes in Pbl2 and perovskite thin films [2]

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.

In our present work we have prepared perovskite thin films with an established 2-step synthesis method that has led to highly efficient solar cells [1]. It comprises the deposition of a precursor layer (Pbl<sub>2</sub>) from solution by spin-coating and the subsequent conversion to perovskite by dipping into a solution containing a

mixture of methylammonium halide salts (MAI and MACI). We have investigated both films with grazing incidence small angle X-ray scattering (GISAXS) and modeled the scattering data within a distorted wave born approximation (DWBA) using three from factors (FF) [2]. We observe a strong correlation of lateral crystal sizes before and after conversion which we attribute to constrained crystal growth. Additionally, by contemplating the intensities of individual FF, we find an accumulation of smaller crystals within the film in contrast to the surface (Figure 1) 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 special confinement (Figure 2).



Figure 2: Proposed mechanism of 2-step perovskite conversion method [2]

Thus, our results shed light on the conversion process itself and can be useful to understand and further improve a range of 2-step methods, which may eventually lead to reproducible high PCE.

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### V<sub>2</sub>O<sub>5</sub> prepared by different synthetic routes as cathode active material for Na<sup>+</sup> and Mg<sup>2+</sup>-ion batteries

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Reducing the costs and improving the performance of batteries for electrical vehicles as well as for stationary applications is the scope of intensive research in the past years. Lithium-ion batteries are still frontrunner for mobile applications and in transport, but with a clear necessity for further improvements [1-3]. An alternative way could be to completely replace lithium and use another metal-ions instead. Magnesium and sodium ion batteries have been already suggested as possible alternative [4], but these are not yet competitive with respect to energy and power density. Li+-, Na+- and Mg2+-ions differ in size, charge, and chemical properties. Therefore it is not by default that the same or analogous host materials suitable for Li<sup>+</sup>-ion intercalation are appropriate for Na<sup>+</sup>- and Mg<sup>2+</sup>-ions as well. The cathode material V<sub>2</sub>O<sub>5</sub> has already shown good performance for Mg<sup>2+</sup> and Na<sup>+</sup> ions and has been recognized as a promising electrode material [5].



Figure 1: Morphology of hollow V<sub>2</sub>O<sub>5</sub>E

The intercalation process, especially its kinetics, is known to be severely influenced by the morphology of the host material. With the aim to synthesize an optimal cathode material based on V<sub>2</sub>O<sub>5</sub>, several synthetic routes, including sonochemical modification of commercial V2O5 powder, anodization of V metal electrochemical deposition and solvothermal synthesis were applied. Scanning electron microscopy, X-ray diffraction and X-ray photoelectron spectroscopy were used for characterization of morphology, structure and composition. V<sub>2</sub>O<sub>5</sub>-nanofibers were obtained by the sonochemical treatment and electrochemical deposition, V<sub>2</sub>O<sub>5</sub>-nanotubes by the anodization method and hollow nanospheres and nanoneedles of V<sub>2</sub>O<sub>5</sub> by the solvothermal synthesis. Cyclic voltammetry, the

potentiostatic intermittent titration technique (PITT) and galvanostatic charge/discharge cycles were conducted to study the intercalation process of the obtained materials in different electrolytes. The intercalation behavior of the V<sub>2</sub>O<sub>5</sub> (VO<sub>x</sub>) materials in different electrolytes are compared to each other. Hollow nanospheres of V<sub>2</sub>O<sub>5</sub> showed the most promising performance for the intercalation of Na ions.

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# Hydrogen dynamics in $\beta$ -Mg(BH<sub>4</sub>)<sub>2</sub> in the picosecond timescale

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Among the complex hydrides, magnesium borohydride is attractive due to a quite good thermodynamic stability and high hydrogen storage capacity (14.9 H<sub>2</sub> wt %).

However, Mg(BH<sub>4</sub>)<sub>2</sub> decomposes only at 600 K and its limited reversibility make it unsuitable for practical application so far. Mg(BH<sub>4</sub>)<sub>2</sub> has been subject of extensive theoretical calculations to understand the ground state of the material and for predicting reaction enthalpies for the various decomposition steps of the hydrogen release.

Different decomposition processes have been predicted and experiments in different pressure and temperature conditions have been performed, showing complicated decomposition pathways. In this framework, the dynamics of the [BH4] units might play an important role, as suggested for other borohydrides.

Quasielastic neutron scattering (QENS) has been performed beta phase of Mg(<sup>11</sup>BH<sub>4</sub>)<sub>2</sub> at the cold neutron time-of-flight spectrometer TOFTOF at FRM II, Munich. Spectra were reordered in the range of temperature from 11 to 500 K.

At low temperature a strong inelastic contribution has been observed, whereas at higher temperatures the quasielastic contribution is predominating.

A jump rotation dynamic has been identified, superimposed to a vibrational dynamic of the entire [BH<sub>4</sub>] units.

The quasielastic signal, as well as the vibrational signal, have been evaluated and used to determine the hydrogen motion in the scanned range of temperature and in the picoseconds time scale.



Figure 1: Elastic Incoherent Structure Factor reordered at 2.5 Å.



Figure 2: Quasielastic spectra reordered at 11 K (grey line), 100 K (blue), 200 K (green), 500 K (red).

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## Spray deposition of titania films with incorporated crystalline nanoparticles for all-solid-state dyesensitized solar cells

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With the invention of conducting polymers, fully organic solar cells and hybrid solar cells combining organic and inorganic materials have drawn a great deal of attention in research since then. Compared to fully organic solar cells, hybrid solar cells have combined advantages of both organic and inorganic components, such as good physical and chemical stability, high electron and hole mobility, high electron affinity, controllable morphology, and well-defined nanostructures. Titania, a n-type semiconductor, has been intensively investigated as the electron-transporting material of hybrid solar cells over last decades. For solar cell applications, a large surface-to-volume ratio of the inorganic semiconductor is desirable, since the morphology influences charge carrier transport routes and the excition dissociation which occurs at the interface of the inorganic and the organic parts, therewith the probabilities of electron-hole recombination. As a result, mesoporous anatase titania films favour photovoltaic activity. In order to obtain more efficient titania photoanodes, we introduce pre-synthesized crystalline titania nanoparticles with a size of 5 – 6 nm into mesoporous titania films.

Sol-gel synthesis in combination with amphiphilic copolymer templates is a promising route for fabrication of porous and nanocrystallized titania nanostructures at room temperature. In this approach, the reactants can be mixed uniformly at the molecular level; the micro-phase separation could take place through a so-called good-poor solvent pair, which induces a large specific surface area after removal of the templates. Meanwhile, the use of diblock copolymer templates in sol-gel synthesis enables the control of the nanostructure and stimulates the formation of an interconnected 2.0

network with tunable porosity and pore size.

Spray coating, a simple and low-cost technique for large-scale film deposition, is employed to fabricate mesoporous titania films in the present work. The surface and inner morphologies were probed with scanning electron microscopy (SEM) measurements and grazing incidence small angle X-ray scattering (GISAXS) measurements, respectively; The polymorph was investigated by x-ray diffraction measurements (XRD). All-solid-state dyesensitized solar cell, whose active laver includes а nanostructured titania film (n-TiO2) with incorporated presynthesized crystalline nanoparticles as an n-type semiconductor, a metal-free dye D149 as a light harvester and P3HT as a holetransporting material (HTM), obtained a high short-circuit current density (Jsc) of 10.0±0.4 mA cm-2 and reasonable power conversion efficiency (PCE) of 2.7±0.1 %.



Figures: SEM image (a) and 2D GISAXS data (b) of spray-coated mesoporous titania film after calcination at 500 °C. Sketch of all-solidstate dye-sensitized solar cell (c).

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### **QuadRad - Muscle-Electrically Powered Vehicles**

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Besides walking, cycling and public transport, there is a great need for personal mobility in Europe. Half of the Europeans use a car every day, which is more than the proportion who cycle (12%) or use public transport (16%) combined [Eur13]. Currently, conventional cars from M1-category (according to the EU-Classification) are used to cover this need. That means, a vehicle with a mass between 1000 kg and 2000 kg is used to transport only 100 kg to 200 kg. Since the mass-ratio between the mean of transportation and transported object is high, this mobility mode is inefficient; regardless of how efficient the vehicle is. Assuming a driver weighs 80 kg and carries goods with a weight of 100 kg with him, arises a mass ratio of 5.5 while using a conventional passenger vehicle with a weight of 1000 kg. However using the QuadRad, with a vehicle weight of 60 kg, as means of transportation the mass ratio is 0.3. With regard to issues such as CO<sub>2</sub> reduction and environmental protection, the trend is towards smaller and alternative vehicle concepts.



Figure 1: QuadRad - Prototype

The so called "QuadRad" is a type of bicycle with four wheels and electric pedal assistance (see figure 1). The vehicle concept is designed especially for commercial applications. Research in the field of courier services have shown that the use of electric cargo bikes against cars or bicycles is more economical. Through use of a pedelec engine the annual mileage of bicycles can be increased by a factor of 1.8. Due to this, the higher vehicle costs can be compensated effortlessly. With the same mileage, an electric cargo bike is more profitable than a car [Gru13]. Compared to a conventional bicycle or cargo tricycle the QuadRad offers a large transport capacity, with a significantly higher driving comfort and simultaneously increased security.

The vehicle concept is powered by a mid-engine with a power of 250 W and a maximum torgue of 70 Nm. In addition to that, the driver is supported up to a speed of 25 km/h from the electric motor, thus the QuadRad does not require registration [Stv13], [Nn02]. The battery module consists of 96 Li-lon cells of type 18650 with a voltage of 44.4 V and a capacity of 1.0 kWh. The maximum electric range is, under ideal conditions, about 90 km.

Overall vehicle weight is 60 kg and the chassis is designed for an additional load of 180 kg. This is ensured by a double-wishbone suspension front and a rigid axle rear. The turning circle is 4 m at a steering angle at the wheel of 39.5°. Moreover, the front pitch of spring is 80 mm (compression: 60 mm; rebounding 20 mm), and, on the rear axle the pitch is only 60 mm (compression: 40 mm; rebounding 20 mm), which is adequate for a vehicle that is used mainly in urban areas [Bor14], [Zie14].

A modular system reduces complexity on the one hand by decreasing the number of parts and on the other hand by the use of common parts. In addition to that, the QuadRad consists of 6 modules, front axle, rear axle, front end and rear frame and the drivetrain (see figure 2). These modules are themselves divided into sub-modules. Due to the modular design, the transport surface can be customized depending on the application.



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# Degradation in printed polymer:fullerene thin films for organic photovoltaics

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Clean and renewable energy sources gain more and more importance. Among them, solar energy has the largest growth potential. In comparison to conventional silicon based solar cells, organic photovoltaics (OPVs) offer several advantages, such as ease of production and a high versatility. Nevertheless, their efficiency is still much below that of conventional solar cells. Up to now, OPVs reach a maximum efficiency



Figure 1: Printing machine

of slightly over 10 %, compared to an efficiency of above 20 % in case of conventional photovoltaics. A problem of OPVs is the degradation of the active layer, which lowers the efficiency with time. Hence, the lifetime needs to be prolonged, so that a profitable large-scale production becomes feasible. Therefore, a detailed understanding of the degradation mechanisms is necessary.

The possibility of printing OPVs enables large-scale fabrication, e.g. by roll-to-roll-fabrication, in contrast to other production methods, like spin-coating. A lot of research has already been done with OPVs produced by spin-coating. However, it is not clear how the method of film application affects the aging behavior.

In the present investigation, we address UV induced aging of PCPDTBT:PC71BM and P3HT:PCBM active layers printed in a positive shim mask slot dye coater (Figure 1). We investigate the influence of this production technique on the morphology and the aging behavior of the active layer, in comparison to that of spin- or spray-coated OPVs. Changes in the morphology of the films due to accelerated aging are investigated by means of optical microscopy, atomic force microscopy (AFM), X-ray reflectivity (XRR), UV/Visible light spectroscopy (UV/Vis) and Fourier transform infrared spectroscopy (FTIR).

By these methods, changes in the crystalline structure, as well as in the chemical structure, i. e. of molecule groups or single atoms, of the active layer film (Figure 2), can be investigated. The understanding of the degradation mechanisms in the active layer, that is caused predominantly by UVradiation in the sunlight, oxygen and water, could eventually help to find polymer:fullerene blends with maximal durability. This will be crucial for a largescale application of this technology.



Figure 2: Polymer:fullerene film printed on glass substrate

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### Foam-like structure of spray coated titania films for photovoltaic application

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Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics. Controlling the pore size is crucial for the photovoltaic applications, such as dye-sensitized solar cells (DSSCs) and solid state solar cells. In this study, spray coating is used, which is scale-up deposition method. In general, spray coating allows for a layer-by-layer deposition, which involves 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  $\alpha_i$  and the exit angle of the scattered X-ray beam (k<sub>f</sub>) is  $\alpha_f$ . A beam stop is placed on the specular beam position.

The third-generation synchrotron source is used, therefore we can obtain a sub-second time resolution with excellent statistics scattering signals. From the 2D GISAXS scattering pattern, the size, shape and amorphous arrangement of titania nanoparticles can be obtained after analysis, which renders in situ GISAXS a powerful tool

characterize to the evolution nanostructures during the spray process. The in situ spray coating GISAXS experiment indicates that the evaporation of the solvent and film stacking mainly influence the structure sizes.

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 realspace 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).



of Figure 2. a) Full real-time mapping of horizontal cuts collected from in situ GISAXS data at qz = 0.35 nm<sup>-1</sup>. 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.

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# Tin oxide Thin Film Reduction via the Polyol Method

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Besides the various physical and chemical processes used for the preparation of metallic Nano-powders ( electrolysis, reduction by hydrogen or hydride), the polyol method displays lots of advantages like acting not only as a reducing agent, but also as a stabilizer or capping agent to stop nanoparticle agglomeration. Over the past two decades, the polyol method has been used in the preparation of nanoparticles such as Co. Ni. Cu, Sn, Ag, Au, Pd, etc. [1]

In a polyol method, the metal precursor can be oxides, hydroxides, nitrates, and acetates that are either dissolved or suspended in the solvent like ethylene glycol (EG). In case of oxide or hydroxide precursors, they have to be at least slightly soluble in EG at high temperature, otherwise, the addition of an acid is needed.

Despite an impressive number of studies made to this synthetic route, it still remains empirical and, to our knowledge, no successful approach has been made in order to investigate the reduction of oxide thin films on solid surface. In our work, we investigated the reduction of Sn oxide thin film [2] on a Sn metal substrate. The reduction of the Sn oxide thin film on a Sn metal substrate was indicated by the abrupt change in the Sn electrode potential when measured vs. a reference electrode (Ag/AgCl). Fig. 1 shows a typical OCP (open circuit potential) measured during heating and cooling cycles of hydrazine-containing ethylene glycol. The sudden change of the OCP at ~102°C corresponds to the reduction of the Sn oxide film as the interface changes from SnO2/EG to Sn/EG. More details about the origin of this OCP change will be provided in the presentation with the help of information obtained from Cyclic Voltammetry (CV).



Fig. 1: OCP of tin wire vs. reference electrode (Ag/AgCl) measured during heating and cooling cycles of hydrazine and LiTFSi-containing ethylene glycol. The sudden potential drop corresponds to the reduction of oxide thin film on the tin surface

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### Silicon/Graphite-Composites as High Capacity Anodes for Next Generation Li-Ion Batteries

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The range of average electrified vehicles is limited nowadays to approximately 150 to 200 km. According to road maps of automotive companies the range of electrified vehicles should be increased by a factor of 2 to 3, within the next decade. In order to reach this aim new active materials are required to get higher specific capacities and lower battery weights, therefore silicon is quite a suitable material for next generation anodes. Silicon has high earth abundance and is not toxic and it has a high specific capacity of 3589 mAh/g according to the metastable Li<sub>15</sub>Si<sub>4</sub> phase. Although these properties should make silicon suitable for battery applications, there are still barriers that have to be overcome to apply silicon as anode material. Hereby the main problem is the large volume expansion of 300-400% between silicon and Li<sub>15</sub>Si<sub>4</sub>, which results in strain and cracking of the Si-particles. This volume expansion is caused by the fact that silicon is not an intercalation material (as graphite is), rather it is a real alloying material.

We demonstrate the influence of different binders, different silicon contents and different silicon particle sizes on the cycling performance and the mechanical properties of pure silicon and silicon/graphite anodes. Therefore water based graphite anodes were investigated and optimized, and then the silicon content was increased step by step. Afterwards the silicon/graphite coatings were optimized in terms of capacity, cycling behavior and mechanical properties. In addition the influence of electrolyte additives on the capacity and the cycling stability was investigated. In Figure 1 the cycling behavior of a water-based nano-silicon anode (Si 100nm, VGCF-carbon fibers, LiPAA-Binder wt% 40-40-20) is shown, in Figure 2 the associated potential curves for the first cycle are depicted. The specific capacity is quite stable at around 950 mAh/g<sub>coating</sub> for about 25 cycles at a C-rate of C/3 and area capacity reaches nearly 4 mAh/cm<sup>2</sup>. The electrode materials are characterized by galvanostatic cycling, impedance measurements, scanning electron microscopy and mechanical testing (e.g. bend test from 6mm to 1.6mm rods). As long-term aim of this project the coating of silicon/graphite composite electrodes should be scaled-up at the iwb at TUM in Garching and tested in 5 Ah pouch cells.



Fig. 1: Specific capacity of a silicon electrode. The values were obtained as the average out of two cells. The cycling was performed in coin cells with lithium as counter electrode.

Fig. 2: Voltage profile of the first cycle. The discharge shows the lithiation of silicon to Li15Si4 which is close to 0 V. The area capacities were 3.89 and 3.63 mAh/cm2, with an electrode area of 1.54 cm2.

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# Model-based operating strategies for chillers with thermal energy storage in Smart grids

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The integration of fluctuating, intermittent renewable energy sources into the power grid requires measures for stable and economical power supply. Multi modal energy systems combine some of the commonly



Figure 1: Research focus within the context of multi modal energy systems

mentioned measures, such as sector coupling, energy storages, or flexible demand.

In cooling-dominated climates air-conditioning of buildings accounts for a large share of the peak load and the overall power consumption. In those climates, demand side management of cooling loads could help integrating larger shares of renewable into the grid. Especially in densely-populated cities energy-dense and cheap ice storages can decouple electrical demand and thermal (cooling) supply. Cooling system operators could benefit from fluctuations in price (arbitrage) and charge or discharge their thermal energy storage.

In this PhD work, an experimental cooling system

consisting of a two-stage compression chiller, cooling fans, and an ice-on-coil type ice storage was thoroughly tested. Based on these tests, semi-

empirical system models were developed. Simulation results show good agreement with independently acquired experimental data, and the models require low computational effort. Based on these models an operation manager (OM, model-based predictive controller) was developed. The OM uses electricity price predictions and weather forecasts to determine (cost-) optimal operating strategies under a given, deterministic cooling load.

In a scenario analysis for a typical hotel cooling load on a summer day in Munich in 2014 two conventional (heuristic) operating strategies were compared to the OM strategy. The first heuristic strategy, state-of-charge (SOC)-controlled chiller operation, is neither able to react on electricity price signals, nor it can consider chiller start-up costs. An alternative heuristic strategy, price-controlled chiller operation, does react on fluctuations in the electricity price. However, since start-up costs are not included in this simple strategy, fluctuations in the electricity price can lead to an unnecessary high amount of chiller start-ups. The OM, on the other hands, accounts for operating constraints (i.e. chiller and ice storage operating limits), price fluctuations, and ambient weather conditions. For the particular scenario



Figure 2: Cooling system architecture

day, the OM is app. 11% and 62% cheaper than the SOC-controlled and price-controlled strategy, respectively.

The introduced cooling system OM may help integrating larger shares of renewables into the power grid. Future research will focus on better strategies for determining the final SOC of a given period. Also, research will focus on the integration of such system into a Smart district cooling grid.

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### **Evolution of the Structure during Functional Stacks Build-up of Inverted Organic Solar Cells**

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Over the last few decades, energy source such as sun, wind and biomass have attracted intensively attention, with the purpose of increasing energy production from renewables. Each of these energy sources provides its own advantages. Solar energy can be strongly utilized in areas of intense sunlight. As reported, the energy from sun irradiation in the earth strongly exceeds the consumption by the whole world. Nowadays, traditional silicon-based solar panels are till the mostly used commercial products in photovoltaics due to its high photocurrent conversion efficiency (PCE), long life time and mature production technologies. However, due to the limits of the application for low-cost, light weight, flexibility and easy production methods, the new generation photovoltaics, organic solar cells, are of great interests. Compared to traditional silicon-based solar cells, lower PCE and shorter life time are the most serious issues to be conquered for organic solar cells. Massive researches on developing new organic materials systems or designing new architectures have been going on, which make their photovoltaic performance much closer to silicon based solar cells.

As is known, the main functional layer of organic solar cells is the active layer, including the donor and acceptor materials. The phase separation between these two materials plays the most important role. The interpenetrating phase of donor-acceptor network in bulk film, denoted as bulk heterojunction (BHJ) film, shows the highest efficiency. The most frequently used geometry for an organic solar cell is the standard geometry, where the positive charge carriers flow from the donor material to the bottom electrode and the negative charge carriers transfer to the top electrode. Today, the poly(3-hexylthiophene-2,5-diyl) (P3HT):phenyl-C61-butyric acid methyl ester (PCBM) BHJ organic solar cells with a standard geometry is the mostly studied system, used to investigate the structure-property relationships.



In this work, we demonstrate that the PCE of the P3HT:PCBM BHJ solar cells can be improved from 3.3% (with standard geometry) to 4.4% by introducing a simple inverted geometry. In the inverted geometry, the charge carrier collection is in an opposite way as compared to the standard geometry. Moreover, it is found that the solar cells show 88% PCE preserved after more than 150 days, if they are not operated continuously. In order to obtain the fundamental understanding of the improvement in PCE and stability, the gradual development of the P3HT:PCBM BHJ morphology in inverted solar cell is examined by AFM and GISAXS measurements during functional stack build-up. The scheme of the functional layer stacks are shown in Figure 1. They are named from S1 to S7 on the basis of the preparation route. Herein, the relationship between the high device performance and the inner morphologies of each functional stack is investigated and compared to the previously measured standard geometry.

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# Life cycle energy factor / life cycle emission factor to assess buildings holistically

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The life cycle energy factor / life cycle emission factor (fLCE) is a method to assess buildings more holistically, over the production, use and disposal phase. Given that the building sector requires a large amount of resources, well-designed buildings can save resources.

The impact of construction and demolition in the building life cycle is higher, due to the increased energy savings during operation. This issue is reinforced through the fact that only nearly zero-energy buildings may be built after 2020 to European Union guidelines.

The embodied energy (EE) is often expressed as a percentage relative to the life cycle energy (LCE), i.e., EE / LCE in %. However, a calculation for plus-energy buildings is sometimes not possible or meaningful (LCE as denominator is 0 or <0). Therefore, a life cycle energy factor / life cycle emission factor ( $f_{LCE}$ ) is suggested in Figure 1. Thereby,  $f_{LCE} > 1$  means that the operation phase dominates;  $f_{LCE} = 1$  represents that the embodied energy and the operating energy is equal over the building life cycle; f<sub>LCE</sub> between 0 and 1 shows that the building materials are responsible for



Figure 1: Definition of the life cycle energy factor / life cycle emission factor (f<sub>LCE</sub>)

more than 50% of the life cycle;  $f_{LCE} = 0$  indicates a zero-energy building (OE = 0);  $f_{LCE} < 0$  and > -1 means that the embodied energy is partly compensated by the operating energy;  $f_{LCE} = -1$  represents a zero-lifecycle-energy building (LCE = 0); f<sub>LCE</sub> < -1 indicates an energy surplus over the life cycle. The f<sub>LCE</sub> is

applicable for all building standards, i.e., from standard buildings (Figure 2, left) to plus-energy buildings (Figure 2, right). In addition, f<sub>LCE</sub> is practical and transferable for emissions, e.g., zero-CO<sub>2</sub> buildings.

It should be noted that an exclusive assessment through the fLCE is insufficient. For example, an f<sub>LCE</sub> value of 0 indicates that the building is a zero-energy building, but this does not necessarily reflect on the building's efficiency; the life cycle energy is variable. Therefore, the whole life cycle should be crucial for the assessment.

The  $f_{LCE}$  extends the commonly used approach; it is possible to rank different building standards and to assess the embodied energy and emissions, respectively.



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### Identifying the key impact parameters for economic competitiveness of Power-to-Fuel

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The need in reducing the global CO2 emissions has already led to a significant increasing share of renewable energies in power generation. Yet, their volatile electricity generation requires flexible storage and power consumers. Besides the electricity sector, the share of renewables in mobility, heat supply and chemical industries has to increase to lower the CO2 emissions in these fields, too. Therefore the conversation of electrical power into fuels - so called Power-to-Fuel - has big potential. Thereby hydrogen is generated out of water by using electrical power during the electrolysis. If this fuel isn't used directly, it could be processed to synthetic hydrocarbons such as methane or methanol in a second process, the Synthesis Reaction.

All of these three different process products have to face intense market competition. The synthetic hydrogen has to compete with hydrogen, which is generated out of natural gas by steam-reforming, the synthetic methane with natural gas and the liquid hydrocarbons like methanol with fossil fuels out of oil. Especially the generation costs of synthetic methane are distinctly higher than the costs for conventionally extracted natural gas currently.

To evaluate the future market shares of these synthetic fuels there are needed models for differing regions like South-East-Asia or Europe. These exposed regions differ in relevant frameworks that both could push or slow down the market penetration of synthetic fuels such as existence of natural resources, geographical position and the resulting trading possibilities for fuels, their sources and costs of power generation, level of technology and industrialization and their already existing infrastructure for fuels. The model's results will show, which frameworks affect the development of synthetic fuels in which way.

However, reasonable parameters are needed for the model's differing scenarios. To define, which technological, economic and regulatory parameters are needed to be varied for this, there has to be done a sensitivity analysis for the generation costs of synthetic fuels before. Out of these results, the key impact parameters on the generation costs can be identified and used for the differing scenarios in the later model.



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## **Optimization techniques for power generation from** waste heat using thermoacoustic engines

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Figure 1: Test rig at the institute

Thermoacoustic engines are robust and simple devices in which heat energy is transformed into fluctuations of fluid pressure and velocity. Those fluctuations carry acoustic energy, which can be transformed into electrical power e. g. by a piezoelectric generator or a piston. Thermoacoustic devices should be robust and cost effective and suitable to recover waste heat at low temperature levels, which would otherwise be discarded.

Thermoacoustic devices can be built with very few moving parts. The geometry is usually rather simple and consists of standard components like pipes and heat exchangers (figure 1). However, the design of such devices is not straight forward and requires tools capable of handling acoustics. This is one of the main reasons why those devices are mainly used in special applications and have not yet found a wider use in industry.

The key part in a thermoacoustic engine is the "stack" or "regenerator". In order to effectively drive the acoustics, a porous solid enlarging the surface area, where an acoustic boundary layer exists and heat transfer takes place, is used to convert heat into acoustic fluctuations. This heat transfer is facilitated by two heat exchangers creating a temperature gradient across the porous medium. The device is acoustically unstable, so that small fluctuations in pressure and velocity of the working fluid are amplified to high amplitudes.

Developing calculation methods and design tools is key to successfully apply these devices. Usually, the thermoacoustic behavior is represented as the scattering matrix of a two-port relating the incident sound waves to the outgoing sound waves at both ports. In other words: the scattering matrix contains



Figure 2: Representation of the low order network. Each box is described by its scattering matrix.

information about transmission and reflection of the stack. This scattering matrix can be used in low order networks (figure 2) facilitating design and calculation taking advantage of the "divide and conquer" principle.



Figure 3: Potentiality: Eigenvalues of the system vs Womersley number (frequency)

In this presentation, a model for the calculation of the scattering matrix explicitly accounting for mean flow through the device is shown. The model is derived analytically from first principles e. g. the Navier-Stokes equations and compared to existing implicit methods and CFD simulations. To post process the CFD simulations, state of the art system identification techniques were used.

In addition, an expression for the instability potentiality – the maximum possible amplification of acoustic wave energy – of a stack is derived from the scattering matrix in order to predict the favorable high amplitudes (figure 3). Here, the eigenvalues of the scattering matrix are calculated and processed such that values larger than unity denote the potential for

instability, while values smaller than unity suggest damping. With this approach it is possible to characterize the stack without knowing of the complete setup, e. g. the boundary conditions.

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# **Enriching Semantic 3D City Models by** Solar Energy Potentials for Wall and Roof Surfaces

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Semantic 3D city models are becoming increasingly available for entire cities like Singapore, Toronto, Rotterdam, Zürich, Helsinki, Paris, Berlin, and even entire countries like Germany and The Netherlands according to the international CityGML standard. In this contribution, I present a method for estimating the solar energy potential (diffuse and direct radiation) for all wall and roof surfaces of every single building within a 3D city model of an arbitrary size that is structured according to the CityGML standard. The specific geographic global radiation values are considered as well as shadowing effects. I will also show how CityGML city models can be enriched by the results of this solar potential analysis.

To estimate the solar energy potential, the following calculations and simplifications are applied: A transition model is used to determine the amount of diffuse and direct irradiation for discrete points in time. For those points in time, the position of the sun is calculated and approximated by a point. The sky, which scatters diffuse radiation to the Earth's surface, is modelled by a hemisphere which is approximated by a set of single points spread on a wide-scaled half-dome. The specific distribution of diffuse solar irradiation from the different zones of the sky hemisphere is considered. All boundary surfaces of the building are sampled to building points in a regular grid. Each building point represents a part of the corresponding surface. By generating intervisibility lines between each building point and each hemisphere/sun point and checking these 3D lines for intersections with the surrounding topography, shadowing effects on the building points are simulated. Based on the information about shadowing the sky view factor (SVF), direct, diffuse and global irradiation is computed for each building point (see figure) and aggregated on the boundary surface and on the building level. The aggregated results are used for enriching the boundary surface objects (roof surfaces, wall surfaces) and stored for further visualization and querying within a 3D-geodatabase (www.3dcitydb.org).



Figure 1: Direct radiation in Dezember - Berlin, Prenzlauer Berg

In a number of projects (e.g. the Energy Atlas Berlin), 3D city models have been used already to estimate the energy demands according to DIN V 18599 for individual buildings. Thus, the estimated solar energy potential can now be compared to the energy demand on the single building level and can be aggregated to districts and up to the entire city. The enriched city model can be used for energy planning as it allows, for example, selecting all buildings a) with roof and/or wall surface area bigger than x sqm, b) with an estimated solar energy potential greater than y, and c) which are not marked as historical monuments. By performing this guery all buildings, which might be appropriate for installing solar panels for energy production can be selected. Analyses of such kind could be embedded into urban planning and building construction for entire cities. The visualization of the city model and thematic queries is performed by using a standard web browser using WebGL and HTML5 technology.

In the presentation I will show the main challenges, the schema for the enriched city models, and give a live demo on how to easily query on the enriched city model as indicated in the example above.

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CPG Center for Power Generation



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