



# **Sustainable Energy Supply of the Future**

**1st Colloquium of the Munich School of Engineering**

18.07.2011



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The Technische Universität München has identified the challenges and tools towards a sustainable energy supply and supports them by virtue of a focused research program. This, we have centered a large range of our activities on the “Green Technologies” in the Munich School of Engineering (MSE).

The MSE is a paradigm for interdisciplinary studies in engineering. Its largest interdisciplinary research project is TUM.Energy to which four research clusters are dedicated: Center for Power Generation, Network for Renewable Energies, Science Center for Electromobility, Centre for Energy Efficient and Sustainable Design and Planning. Up to 100 professors from ten departments are working on the technical challenges of energy research. The first move towards these challenges is the identification and connection of all existing activities at TUM regarding energy research. Therefore, the colloquium „Sustainable Energy Supply of the Future“ was organized to provide insights into the variety of energy research activities at TUM through presentations and posters. Furthermore, the MSE colloquium is one first step to build a platform for interdisciplinary exchange and enables partnerships within TUM and with external partners.

A handwritten signature in blue ink that reads "Wolfgang A. Herrmann". The signature is written in a cursive style.

Wolfgang A. Herrmann  
President

## Center for Power Generation

The Center for Power Generation unites those institutes of the Technische Universität München with research activities in the field of energy conversion for power generation. Besides efficient and innovative power plant technologies, the research spectrum of the CPG includes future systems for transport, energy storage and power plant control as well as new and optimized techniques for the reduction of air and climate pollutants in the energy conversion process.

The first project of the CPG will be the analysis of the energy supply in the city and region of Munich, concerning power generation, electricity transport, distribution and consumption. This analysis should reveal the potential for a future energy supply and the feasibility of the integration of new energy technologies. With the project "TUM.Energy for Munich" the CO<sub>2</sub> emissions of the region of Munich shall be reduced by 80 % compared to the level of 1990 by the year of 2030.

The members of the CPG will there fore focus on four main topics:

- Analysis of the energy supply of Munich and studies for the integration of sustainable and innovative technologies
- Synthetic energy carriers
- Flexible and efficient power plant technologies
- Solarthermal power generation

More than 15 institutes of the faculties of electrical and information technologies, chemistry, mechanical engineering and physics are working together within the CPG to develop new solutions for the energy future of Munich.

## Network for Renewable Energy

The Network for Renewable Energy (NRG) is a network for inter-faculty research at the Technische Universität München consisting of a multitude of different chairs at the TUM which are focussing on the topic of renewable energy.

The network is one of currently four research centres at the Munich School of Engineering. Together, these four centres follow the aim to achieve a sustainable energy supply of the future.

NRG is headed by Professor Müller-Buschbaum, Chair for Functional Materials, and was founded to create the opportunity to stem interdisciplinary, large-scale research projects. Additionally regular meetings within the network take place to foster an active communication between different research groups. There is already an active participation of various disciplines to form the NRG: Physics, Chemistry, Engineering, Electronics and Informatics, as well as the Centre of Life and Food Sciences Weihenstephan, the Walter-Schottky-Institut and the Bavarian Center for applied Energy Research (ZAE Bayern).

The research within the Network for Renewable Energy therefore offers a wide range of topics: from nanoelectronics and material research, as well as microbiology, applied and theoretical chemistry to biomass power stations, wave and solar energy systems, to mention only a few on the steadily growing list.

## Science Center for Electromobility

The Science Center for Electromobility (Wissenschaftszentrum Elektromobilität – WZE) is a union of various research institutions at TUM in which numerous participants from eight different faculties are connected to each other. Thus, a wide spectrum of research is covered ranging from fundamental research on future battery technologies to the applied science on further improvement of components and their integration into an economic and suitable vehicle concept. Furthermore, a direct contact to the industry is established by the creation of the WZE industrial advisory board which enables the mutual coordination of R+D activities. On this basis, extra-ordinary and innovative solutions can be developed that are not limited to the development of electric vehicles but aim on mobility as a whole.

By the integration of the Science Center for Electromobility into the Munich School of Engineering (MSE), the focus level is further extended. Within this frame, electromobility represents a central element to improve the efficiency and sustainability of energy supply and consumption. This technology does not only allow the use of renewable energies for mobility but also extends their usability into other fields of use. Using this integrative approach enables us to develop new solutions and to use them for applications that have only been considered separately until now. To ensure the environmental compatibility and sustainability of mobility and to affect positively other areas of energy use, the Science Center for Electromobility is an important institution of TUM for the energy research of the future.

## Centre for Energy Efficient and Sustainable Design and Building

In Germany, an essential portion of primary energy is consumed by buildings, thus, holding an enormous potential for energy savings that could contribute to reach the demanded climate protection goals. Buildings cannot be reduced to their energy efficiency; moreover, cultural, social and economic aspects have to be taken into consideration. Buildings should provide a comfortable, sustainable living environment and should be designed with the local conditions in mind, such as the climate and its physical and cultural environment.

These complex and interdisciplinary challenge requires new comprehensive solutions. To find solutions for this complex challenge, the Centre was founded with participation of the chairs of Building Physics (Faculty of Civil Engineering and Surveying), Building Climatology and Building Services (Faculty of Architecture) as well as Energy Economics and Application Technology (Department of Electrical Engineering and Information Technology).

The coordination of the Centre is assumed by the Institute of the same name, which was founded under the lead of Prof. Dr.-Ing. Werner Lang. Due to the cross faculty composition of the Centre the expertise reaches from extensive consideration of sustainable urban development and sustainable building to detailed design of energy efficient façade elements and many more aspects related to energy efficiency and the use of renewable energies in building.



## Munich School of Engineering Teaching Department

The Munich School of Engineering (MSE) of the Technische Universität München is based on an innovative concept: the combination of interdisciplinary research and cross-faculty teaching. The teaching department of the Munich School of Engineering (MSE) provides currently two degree courses with the emphasis on an interdisciplinary education in the field of engineering sciences.

Talents in mathematics and science 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.

Since the winter semester of 2010/11, the MSE provides the bachelor course Engineering Science and the master course Industrial Biotechnology:

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.

# Programme

from 8.00 am Registration

**9.00 - 9.30 am**

## Opening

Prof. Lienkamp

**9.30 - 10.45 am**

**Session Chair: Prof. Lienkamp**

### **Sustainable Mobility – Supplying Clean and Affordable Energy for TUM's Electric Vehicle MUTE**

Dipl.-Ing. Gohla-Neudecker, Dipl. Ing. Kandler (Institute for Energy Economics and Application Technology)

### **A Simulation Model for a Smart Home and Vehicle to Building Applications**

Dipl.-Ing. Brendle (Institute of Automotive Technology)

### **Economics of Vehicle-to-Grid**

M. Sc. Ciechanowicz (TUM CREATE)

**10.45 - 11.15 am Break**

**11.15 - 12.30 pm**

**Session Chair: Prof. Lang**

### **Fluidized Glass Façade Elements for an Active Energy Transmission Control**

Dipl.-Ing. (FH) M. Arch. Stopper (Department of Building Climatologie and Building Services, Center for Energy Efficient and Sustainable Design and Building)

### **Research on Mini- and Micro-CHP-Units**

Dipl.-Ing. Sängler (Institute for Energy Economics and Application Technology)

### **Production Based Energy Management Tools for the Food Processing Industry**

Dipl.-Ing. Franke (Chair of Food Packaging Technology)

**12.30 - 12.40 pm**

**Poster Announcement: Prof. Lang**

**12.40 - 2.00 pm**

**Lunch Break/Poster Presentation**

**2.00 - 3.15 pm**

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

### **Green Gasoline Made from Catalytic Conversion of Lignin**

Dr.-Ing. Zhao (Chair for Chemical Technology II)

### **Morphology of Bulk Heterojunction Systems for Polymer-based Photovoltaics**

Dipl.-Phys. Ruderer (Chair of Functional Materials)

### **Photovoltaics of Nanoscale Circuits Comprising Photosynthetic Proteins**

Dr. Holleitner (Walter-Schottky-Institut)

**3.15 - 3.45 pm Break**

**3.45 - 5.00 pm**

**Session Chair: Prof. Spliethoff**

### **Power Storage Requirements for Renewable Energies**

Dipl.-Ing. Tremel (Institute for Energy Systems)

### **Storage of Bio-Energy - Substitute Natural Gas (SNG) as Contribution to Future Energy Systems**

Dipl.-Ing. Fendt (Institute for Energy Systems)

### **Modeling Long-term Impacts of Regulatory Instruments on the German Energy Sector**

Dipl.-Kffr. Hammer (Chair of Management Accounting)

**5.00 - 5.20 pm Break**

**5.20 - 5.50 pm**

**Keynote Speaker: Dr. Christof Spangenberg**

(Director of the K.Group, Munich)

**5.50 - 6.00 pm**

**Closing**

**6.00 pm**

**BBQ**

## **3 Oral Presentations**

# Sustainable Mobility – Supplying Clean and Affordable Energy for TUM’s Electric Vehicle MUTE

Dipl.-Ing. Bodo Gohla-Neudecker<sup>a</sup>, Dipl.-Ing. Christian Kandler<sup>b</sup>, Prof. Dr.rer.nat. Thomas Hamacher<sup>c</sup>

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## Introduction

Oil has become one of the most important factors in international politics. Internal Combustion vehicles are closely tied up with the supply of crude oil, whereas the pictures of empty motorways are impressive examples of this connection. However, the dominance of crude oil in the transport sector complicates the realisation of different environmental policy goals like the reduction of urban pollutant and carbon emissions. Due to this fact, electric vehicles (EVs) such as TUM’s MUTE are currently a hot topic high up on the agenda of politicians, economists, scientists and even the public. Many expectations rest on the economic and ecological impetus, which EVs may bring for the automobile industry of a country. Yet the crucial factor for its success lies with the type of power plants in the upstream energy chain, which de facto determine operation costs and attributed emissions of EVs. It is thus vital to closely screen the true power production costs and CO<sub>2</sub> emissions of power plants, which provide the additional electricity needed to charge potentially several million EVs. In the following paper this questioning with focus on the project MUTE of TU München has been discussed.

Charging TUM’s MUTE with the German grid mix of 2015

When using the overall German Power Plant Mix as a basis for calculating emissions and charging costs, the MUTE is considered and defined as a regular consumer of electricity. No means of smart charging to minimise costs and/or emissions exist. Hereby the total amount of CO<sub>2</sub> emissions and power production costs are equally divided onto the generated kilowatt hours of the whole German grid. The average grid mix for gCO<sub>2</sub>/kWh and for €/kWh can hence be established. Thus emissions and costs are allocated to each individual consumer of electricity according to its very own final energy demand.

The MUTE has a calculated final energy demand (Plug2Wheel) of 7,5 kWh/100km. If the overall German Grid Mix for 2015 (Figure 1, left column) is applied as a basis for calculation, approx. 41 gCO<sub>2</sub> are attributable to the MUTE per kilometre driven. Charging costs for electricity make up about 2,10 €/100km. This amount already includes approx. 40 % of taxes and surcharges as well as additional costs for subsidising renewable energies (“Erneuerbare Energien Gesetz – EEG”) predicted for 2015 for household electricity use in Germany.

The allocation of specific emissions and costs according to this methodology is, however, only accurate for a smaller number of EVs. As soon as several million EVs draw power from the grid, the whole German power generation sector emits considerably more CO<sub>2</sub>, than calculated on an average basis before. This is a direct result of the additional electricity demand required by EVs. In general the final energy demand of EVs is shifted from the transport sector of an economy to the power generation sector. Hence specific power plants are required to produce additional electricity with all its attributed emissions and costs. However, the additional electricity can only be generated by power plants, which are either idle or are not already operating under full load. Methodically these are then the power plants responsible for emissions and costs due to EVs drawing power from the grid.

Cost-efficient charging of the MUTE during off-peak hours

A more accurate allocation of EV emissions and charging cost is based on a detailed analysis of EV charging times and the corresponding power plants generating the additional electricity in a certain hour of day. Figure 1 (right column) displays those power plants ramping up their power generation capacity, when minimum possible charging costs at times of low residual low (off-peak in early morning hours) are aimed for.

Charging costs and attributable emissions for the MUTE hereby amount to approx. 1,30 €/100km and 67 gCO<sub>2</sub>/km. As depicted this is a direct consequence of hard coal and lignite fired power plants, which are the next most cost-efficient power plants in the merit order able to provide the additional electricity required by EVs connected to the grid.

A look at other countries' power generation infrastructure (Figure 2) lays down a varying environmental impact due to the MUTE: An analysis of the French, Swiss and Norwegian power plant infrastructure shows the MUTE responsible for about 3 gCO<sub>2</sub>/km. This is predominantly due to nuclear power plants in France, hydro power plants in Norway and an almost equal mix of nuclear and hydro power in Switzerland. In countries with a power generation infrastructure based mainly on natural gas, such as Italy, California (USA) and Singapore, the MUTE is responsible for approx. 40 gCO<sub>2</sub>/km. Low emissions result from high gas turbine and combined cycle efficiencies as well as from a low specific emission factor of natural gas. In China hard coal fired power plants are used to cover the middle load during off peak hours. Emissions of about 76 gCO<sub>2</sub>/km are hereby attributable to the EVs such as the MUTE. In comparison to Germany emissions are higher due to the less efficient Chinese power plant technology in operation. In countries such as Greece with a predominantly lignite powered infrastructure approx. 85 gCO<sub>2</sub>/km can be considered as a direct result of driving the MUTE. This is mainly due to the high specific emission factor of lignite.

Thus for Germany and China a shift to e-mobility has no immediate environmental benefit; Italy, California and Singapore profit from a slight but noticeable reduction and France, Switzerland and Norway emerge as the major environmental beneficiaries effectively capable of strongly reducing the emissions of the automobile sector in the short term. Yet in summary all considered countries except Norway would be dependant on thermal power plants to provide the additional electricity needed during off-peak EV charging hours. This results in either high or moderate CO<sub>2</sub> yields per km or additional nuclear waste accumulating due to a switch to electric mobility. What is the more sustainable alternative?

#### Charging of MUTE at zero emission level

Another charging option including approximately zero emissions is the direct supply through local integration of renewable energy sources into the complex of a single-family house. According to the requirement of a secured charging of the MUTE - even in periods of renewable stagnation - at maximum a 20% share of electricity purchase from the grid of the hourly charging demand is allowed.

The suburban location, which the simulation is based on by means of specific weather data, is characterized by good PV and rather average wind suitability. The single-family house includes a building area of 120 m<sup>2</sup> and an individual garage with an appropriate charging facility. MUTE is therefore charged using a standardized household socket (maximum charging power 3,7 kW) controlled by load management to get an equalized charging both daily at off-peak periods and during night hours.

Under the assumption of a typical driving purpose as a second vehicle - including an annual distance of 15.600 km and a depreciation period of the renewable energy systems of 15 years - new installation capacities of 9 kW PV (needed roof area 60 m<sup>2</sup>), 2 kW wind power and 2 kWh electrical storage (Lithium-Ion storage) result as a consequence of an hourly based simulation. Figure 3 illustrates the needed high overproduction of the installed overcapacities and furthermore high fed-in tariffs due to the fact of the strict renewable charging criterion (renewable share of the charging demand of 80% in 99% hours a year). As shown, in summer most of the time there is no need for using the electrical storage. On the other hand Figure 4 shows the exemplary coverage of the charging demand during an extreme winter day. This figure also shows the behaviour of the total system at periods of renewable stagnation including high usage of storage and electricity purchase. Figure 5 displays the monthly comparison of renewable electricity production and charging demand on the balance sheet including the already mentioned overproduction of renewable energy systems due to the strict renewable charging criterion.

By maintaining the needed criteria of the simulation annual driving costs of about 50 € result. On the one hand, these costs consist of annual expenses due to infrastructure, maintenance and operation of the renewable energy systems and on the other hand of electricity purchase and renewable fee. On closer examination of the total costs the large share of renewable tariffs for solar produced and either own consumed or fed-in electricity is clearly recognizable. Over the total observation period of 15 years nearly a compensation of the infrastructural costs (~ 23.000 €) by the renewable fed-in tariffs takes place. The electricity purchase from the grid is limited to 13 kWh a year, which has the effect of a very small share of electricity purchasing costs and also of the status of a zero emission charging system. At a direct apportionment of the infrastructural and operational costs to the total renewable produced electricity, direct power generation costs of about 0,12 €/kWh result.

#### Conclusion

The introduction of electric vehicles such as TUM's MUTE into the mass market over the next 10 years poses the question, where EVs will find the most favourable conditions concerning economic and environmental criteria. There is no doubt that low operating costs and environmental implications due to EVs provide the best basis for moving out of the niche

and into the mass market. Hence the crucial factor for a market breakthrough of EVs lies with the type of power plants in the upstream energy chain, which de facto determine operation costs and attributed emissions of EVs. Countries such as France and Switzerland emerge as major environmental beneficiaries effectively capable of strongly reducing the emissions of the automobile sector in the short term. At the same time the additional electricity can be provided by existing nuclear power plants at very competitive costs.

Yet in summary all considered countries would be dependant mainly on middle load thermal power plants to provide the additional electricity needed during off-peak charging hours of the MUTE. This results in either high or moderate CO<sub>2</sub> yields per km or additional nuclear waste accumulating due to a switch to electric mobility. On a long term basis it will therefore become inevitable for the power generation sector to switch to predominantly renewable sources. The long lasting aftermath of CO<sub>2</sub> emissions and nuclear waste attributable to EVs can hereby be avoided. Coupling the power demand of EVs to the fluctuating feed-in of renewable energies thus has a high potential to foster sustainability in both the power generation and the automobile sector. As a result the introduction of electric vehicles has to be combined with the development and expansion of renewable energies at an optimal interaction level.

#### References

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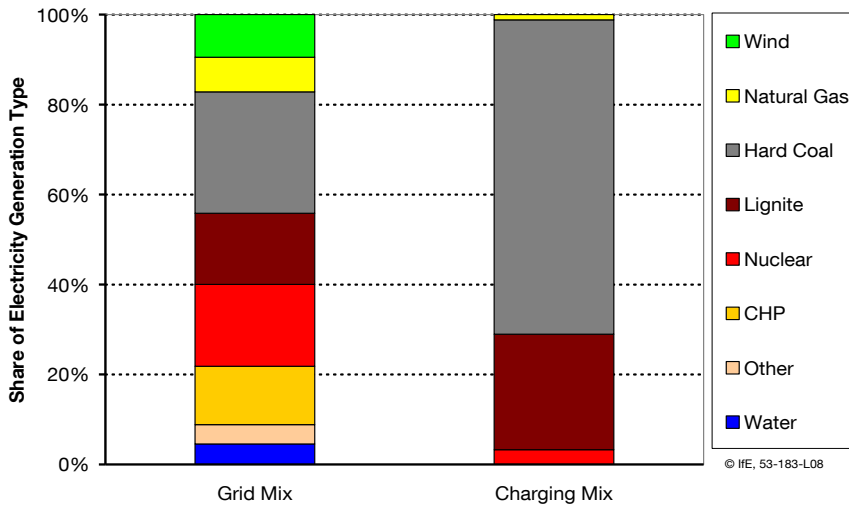


Figure 1: Composition of the MUTE's charging mix in Germany 2015.

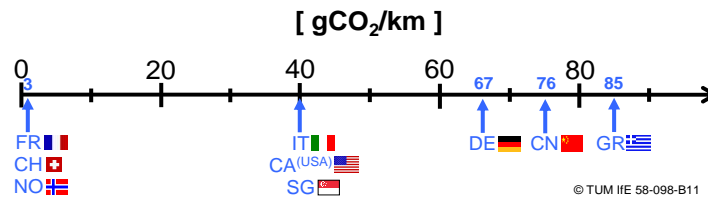


Figure 2: EV emissions scale: Specific CO<sub>2</sub> emissions attributable to the MUTE in various countries 2015.

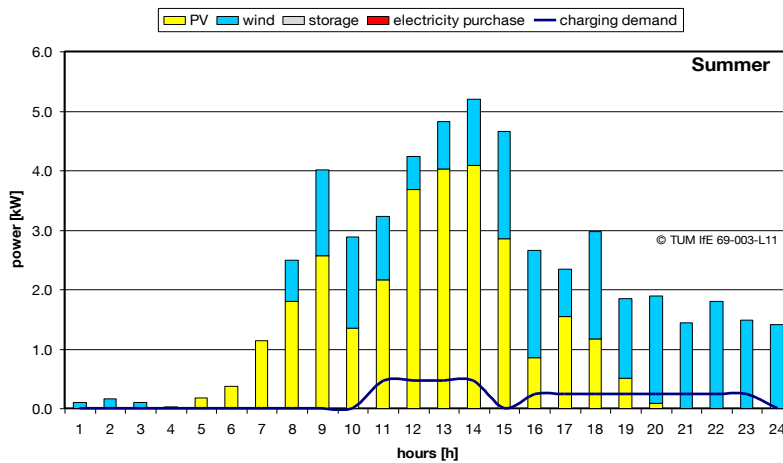


Figure 3: exemplary coverage of the charging demand of the MUTE at a typical day in summer

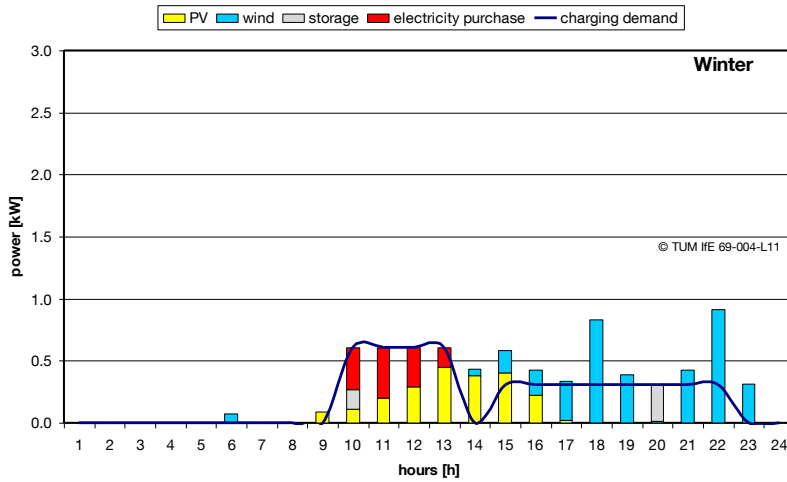


Figure 4: exemplary coverage of the charging demand of the MUTE at a typical day in winter

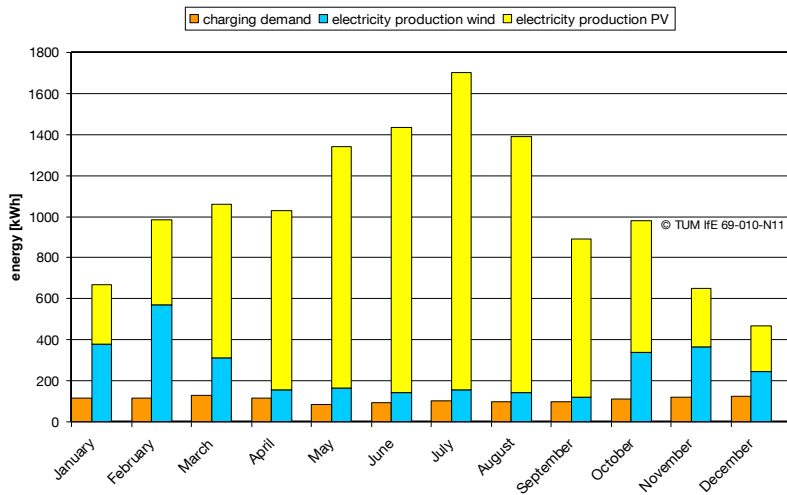


Figure 5: comparison of renewable electricity production and charging demand on the balance sheet



# A simulation model for a smart home and vehicle to building applications

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Topics like the reduction of CO<sub>2</sub> emissions and energy consumption are currently more important than ever before. Particularly in private households innovative heating systems, novel insulating materials and smart high-efficiency electrical consumers are used in order to save energy and reduce greenhouse gas emissions. In parallel, research and development of the automotive industry is working on more efficient automobiles with alternative drive train systems. The target is developing cars with fewer emissions and less energy demand such as hybrid and electric cars which enable driving without local CO<sub>2</sub> emissions.

However, in this regard almost all approaches aim at reducing the energy consumption and the emissions in just one of both fields, “buildings” or “mobility”. By considering both subareas as a combined holistic system, there is further energy saving potential in respect to the total energy demand due to synergetic effects.

Current research projects regarding Smart Homes and Vehicle to Building (V2B) are already combining buildings and vehicles electrically and are integrating electric vehicles into the domestic electric installation. However, the primary goal of these endeavors is to

smooth the load profile on a household level rather than to reduce the individual-related total energy consumption and thereby its CO<sub>2</sub> emissions. This means that by using an intelligent control of charging and discharging of the electric vehicles, the building’s load profile can be adjusted to the electricity supply of the electric utility, the overall energy demand, however, remains equal.

In contrast to this, the present paper aims at sensing possibilities and synergetic effects how the holistic consideration of both elements, “buildings” and “mobility” can contribute to reduce the individual-related total energy consumption. Therefore, a simulation model is presented which emulates the thermal and electric energy demand of a plug in hybrid vehicle and a residential building. The holistic system contains energy sources, energy storages and energy sinks, thermal as well as electric ones. Thus, it is possible to analyze a Smart Home including a vehicle and to detect synergetic effects in respect to minimization of the total energy consumption. Once those effects are detected, a control strategy can be developed focusing on the minimization of the total energy consumption.

# Economics of Vehicle-to-Grid

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Vehicle-to-Grid (V2G) is the concept of buffering energy in the batteries of electric vehicles and feeding it back into the power grid at peak demand times. The need for such a concept is justified by the fact that the power grid offers no inherent energy storage possibility and hence there has to be a fine-tuning of energy demand and supply to keep them equal at all times. Distributed energy storage, as enabled by a large number of EVs, could lower the need of auxiliary, expensive energy production capacities and thus decrease the costs drastically as well as increase the total efficiency of the system.

Figure 1 depicts the V2G concept where energy is produced in power plants and led across maximum, high, medium, and low voltage lines up to the households and/or enterprises and demand-oriented back to the grid. In Figure 2 the steady deviations between demand and supply that occur over a day are shown. A cutout of the range from 13 to 14 o'clock represents the load curve in this period in detail. It is to be recognized that the deviations are not necessarily higher in times of peak load.

The goal of the underlying investigation was to assess the potential economic profit of V2G on different energy markets in Germany like peak or balancing power, using real market data from the year 2009. To this end, the different energy markets were analyzed and a cost model for determining potential profits on these markets was developed. This comprises the definition of

formulas for calculating sales, costs, and profits, and their evaluation on real energy market data. Formula 1 depicts the way total sales can be calculated while formula 2 is the same for the total arising costs.

Based on this approach, a novel software tool named V2G Profit Agent (V2GPA) was developed that allows fast, flexible, and easy-to-use evaluation of different V2G scenarios. V2GPA also supports the search of appropriate values for model parameters, to help assess V2G from the point of view of the consumers and energy companies, respectively. Thus, V2GPA is a valuable tool especially for energy companies to study the potential of V2G and test novel business models related to it.

On the basis of the investigated facts, the achievable profits with V2G shown in Table 1, and the unlikelihood of the best case there has to be retained that for now and in a foreseeable future selling energy in negative direction of energy flow (V2G) only create profits in exceptional cases. In positive energy flow direction (G2V) EVs cannot only be charged for free but instead gain a profit that is between 1.621 and 4.275 € in the market of balancing power in the average case. If negative and positive balancing power cannot or may not be decoupled from each other, there have to be exact analyses under which conditions the combined use is worthwhile. For Example, in the eE-Tour case, a modified average case scenario based on real data from the eE-Tour project, a combined profit of 1.814 € can be gained for MRL.

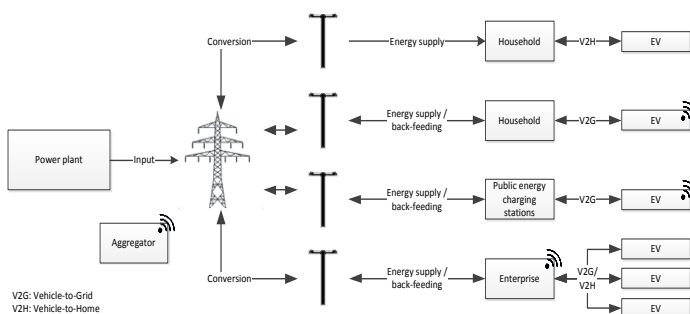


Figure 1: The V2G concept.

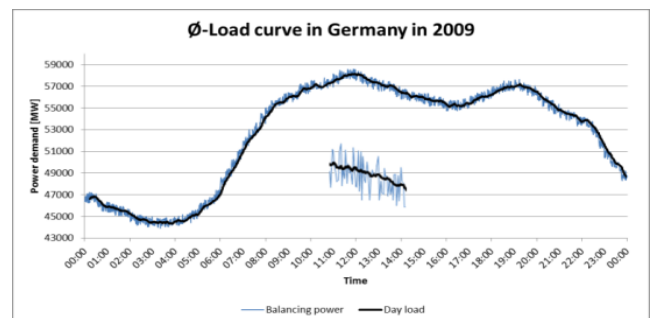


Figure 2: Average load curve in Germany in 2009.

Theoretically, V2G seems to be a feasible solution of balancing demand and supply. Challenges like user acceptance, a change in energy market prices and volumes when introducing V2G on a broad basis, or a tax income reduction when using electricity instead of oil have to be accomplished. In practice, an economic application of V2G fails in most examined scenarios because of a too high ratio of the arising costs to the attainable sales. With over 95% of the total arising costs, the variable costs due to battery wear triggered by each load/unload cycle are the highest cost driver.

The mentioned economical failure of V2G in connection with the necessity of stabilizing the grid makes it inevitable to optimize the way the transportation and the energy sector should be integrated. The transportation sector, consisting of traffic flows and traffic management strategies and the energy supply sector, consisting of management of energy resources and charging strategies inter alia, are more or less separated for the time being. Under the circumstances of a less predictable energy supply market consisting of a much higher fraction of renewable energies, these two sectors have to be integrated intelligently and economically

worthwhile to cope with the challenges of a huge distributed electric vehicle fleet in future.

In further research, we will extend and adapt the developed cost model to the special needs of Singapore. Furthermore, we will develop tools with which it will be possible to study several scenarios for an e-mobility infrastructure with distributed and mobile energy demand and storage capabilities. Applications like driver assistance based on predicted traffic information will be made possible. As the next step, modeling techniques and formalisms will be developed that enable seamless composition and integration of different aspects such as battery behavior, user patterns, and renewable energy sources. Taking into account potential business cases, the overall integration of electric vehicles with the environment via an ICT infrastructure will be covered and a unified approach will be guaranteed. With respect to electric vehicles and infrastructure the whole bidirectional energy supply chain will be modeled.

$$U_{Gas} = \left( \min \left\{ U \cdot I \cdot \sqrt{S}, \frac{(E_{Akku} \cdot T - \frac{d_s + d_p}{F})}{t_A^{max}} \cdot \eta_{el} \right\} \cdot t_L \right) (P_L + P_A \cdot V_{LA})$$

Formula 1: Total sales achievable with V2G.

$$K_{Gas} = L_L \cdot t_L \cdot V_{LA} \cdot \left( \frac{k_E}{\eta_{Umw}} + \frac{K_{Akku}^{fix} + K_{Akku}^{Arbeit}}{Z \cdot E_{Akku} \cdot T} \right) + K_0 \cdot \frac{d}{1 - (1 + d)^{-n}}$$

Formula 2: Total costs of V2G.

Type of load	Profit in the area of... [€]							
	...negative types of load (V2G)				...positive types of load (G2V)			
	Best	Average	Worst	eE-Tour	Best	Average	Worst	eE-Tour
PRL	4.556	-11.437	-48.078	-6.320	20.240	3.327	1.065	3.327
SRL	0	-32.507	-58.455	-20.227	22.932	4.275	765	4.275
MRL	23.627	-2.614	-7.264	-406	12.622	1.621	189	2.220
On-Peak	0	-50.319	-161.313	-66.425	---	---	---	---
Off-Peak	0	-51.283	-163.199	-68.460	---	---	---	---

Table 1: Achievable profits with V2G in Germany in 2009.

# Fluidized glass façade elements for an active energy transmission control

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**Objective:** A glass façade system which controls the energy flows within the transparent building envelope is proposed. The façade enables the perfect comfort in the building, while simultaneously reducing the energy demand. Two fluid filled layers will be implemented in the glass façade. These two layers are regulating all energy flows. The inner fluid layer keeps the surface temperature just below or above room temperature for heating and cooling. The outer liquid layer controls the solar radiation by absorption. The two basic operating modes in summer and winter are illustrated below (Figure 1 & 2).

This system integrates floor heating, cooling ceiling, solar collector, shading device and insulating façade in one element. The transparent façade increases the energy efficiency of buildings in every climate zone and enables the use of renewable solar energy at the whole façade area.

**Methods:** For the proof of concept of the latest developments a new prototype has been build and experimentally tested. The prototype features two fluid layers separated by an insulating glazing. A physical

model of the façade system has been developed and experimentally validated. Buildings equipped with new façade system were simulated in order to determine the performance of the system in different climate zones.

**Results:** The concept of the façade system could be proven with the new prototype. The challenges of handling the static pressure, uniform distribution of the liquid within the layers, and variation of the solar absorbance of the fluid layers are under control. Yearly simulations show the unique behavior of the new façade system.

**Conclusion:** Architects and engineers will receive a standardized product, which increases the efficiency of their building significantly. The user-friendly plug and play system enables the use of renewable energy in an easy way. Because of the active control, the system can be used in every climate zone at every building type.

**Partners:** University of Liechtenstein (project management); Technical University of Munich TUM; Interstate University of Applied Sciences Buchs NTB.

Industrial partners: GlassX AG, Eckelt Glassolutions Saint-Gobain, Hoval AG, and Hilti Corporation.

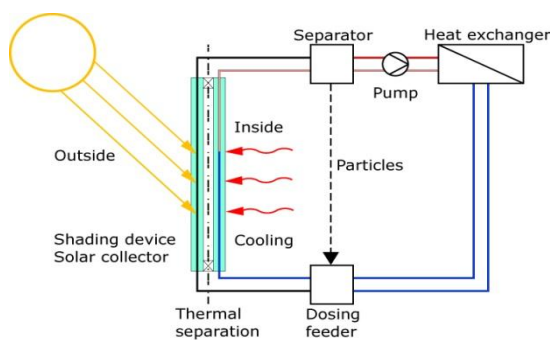


Figure 1: Basic operating modes in summer.

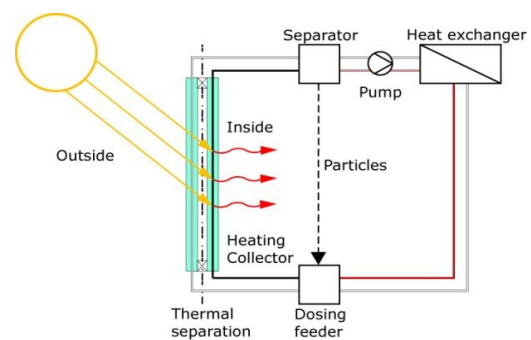


Figure 2: Basic operating modes in winter.

## Research on Mini- and Micro-CHP-Units

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One of the main research topics of the Institute for Energy Economy and Application Technology (IfE) is the analysis of heating systems, especially for residential buildings. For more than ten years, the development of heat demand and heat generation is part of the economical, ecological and experimental research of the Institute. Since 7 years, the main focus of investigations is Combined Heat and Power (CHP) for residential heating purposes. The investigations include theoretical work, experimental work at testbeds, simulations and field tests. The analysed power ratings are Mini-CHP-Units with a power up to 5 kW<sub>el</sub> and 13 kW<sub>th</sub> and Micro-CHP-Units up to 1 kW<sub>el</sub> and 5 kW<sub>th</sub>. The analysed technologies are internal combustion engines, stirling engines and a fuel cell. These units can be used in different sizes of homes from single-family houses up to multi-family houses as well as specific buildings of the trade and commerce sector. For example, hotels or hospitals are suitable for the usage of CHP technologies.

Compared to a separated generation of heat and power the overall efficiency of residential buildings can be increased significantly by CHP systems. As shown in our theoretical work as well as in simulations, the reduction of CO<sub>2</sub>-Emissions and primary energy consumption is highly depending on the reference system. Compared to the existing generation system, a reduction of primary energy usage and CO<sub>2</sub>-Emissions up to 24 % is achievable.

The experimental work at the testbed analyses the control of Mini-CHP-Units in detail. The testbed can simulate dynamic heating conditions in real time. Five so-called Type Days, which represent the seasonal climate in Munich, enable high-precision results of the CHP operation. Using this Type Days the standard control of the CHP-unit was compared to an optimized,

scheduled operation. This research identifies an optimization potential. The knowledge of the state of the typically used thermal storage is very important for an improvement of the control system. Due to this result the "Innovative Heat Storage Management" was developed and tested at IfE. With a more efficient usage of the thermal storage this innovative control allows to increase the onsite generation by switching from Heat Management to Power Management if the storage is in a certain state.

The field tests are mainly focused on different hydraulic integrations and especially on the impact of different buildings and their inhabitants' behaviour on the CHP-operation. The results of the field tests demonstrate, that a high onsite generation is very important for the economic success of a CHP unit. Another very important parameter is the annual operation time of the CHP-Unit. This time can be increased significantly by using an adequate hydraulic scheme with combined heat buffer and a demand adapted CHP unit size.

Upcoming and future research topics are the improvement of CHP-controls and the identification of new applications for CHP-units. The "Innovative Heat Storage Management" is planned to be tested with smaller Micro-CHP-units on our new small scale testbed. Furthermore it will be applied in field tests with Mini- and Micro-CHP-Units. The usage of small CHP-Units in the trade and commerce sector is one of the upcoming research topics. In this field of application the combined production of heat, cold and power is very interesting.

Huge numbers of CHP-units can be used as central part of the future distribution network to form a Smart Grid. Load modulation, according to the electricity demand and the power generation, as well as peak shaving can integrate fluctuating renewable energies.



# Production based Energy management tools for the food processing industry

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The German food industry is divided into 33 branches with 5800 companies overall with an average of 90 employees per company. The energy demand is assumed to be 204 Penta-Joule per year, which means that the food industry is the 6th important energy consumer in the German industry. In addition to optimize single production units, further energy saving concepts should take into account an extended view on the in-plant interdependencies. The still increasing automation level and the computer aided production data acquisition makes the use of simulation techniques feasible, accompanied by data validation. Thus, the objective target of the presented approach is to improve energy efficiency by establishing in-plant management tools for the collection of data, the assessment of the production units and decision support. The basic idea is to merge the production planning with the energy management. To reach this, the approach is subdivided into four steps,

- standardized process description,
- data acquisition and analysis,
- model specification and
- process simulation

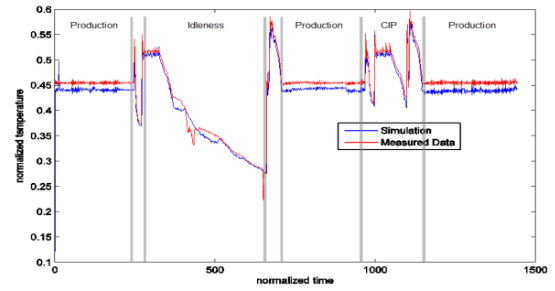
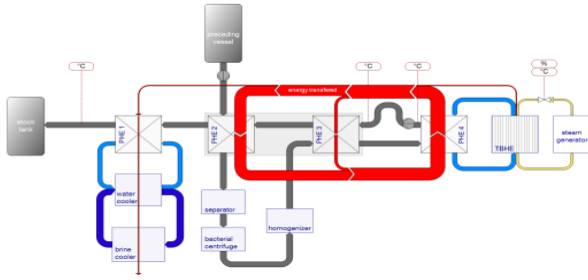
resulting in a validated „virtual plant“. The standardized process description defines the several process units of the plant with a piping and instrumental diagram. It consists of the equipment; the energy based measuring points and the gateways to other units. For the data acquisition and analysis, a process control system delivers the sensor values. (Note that in some cases there is a need to get additional data for a complete energy related description of the production unit, thus additional mobile measurement methods come into

account.) Based on the data analysis energy characteristics suitable for networked factories are applied. The paradigm for the model specification is a set of context free model components. Obviously, Sankey diagrams are well established and suitable for mapping the interrelationships of the energy sinks and sources as well as special process equipment, since the different energies like heat and product flows are represented in one framework. With the help of the process simulation the energy consumption for production schedule of single processes or a greater part of the plant network is predicted according to virtual work orders. The intermediate steps already prepared to the current project are

- as-is-analysis in selected small and medium sized food production enterprises
- model specification and validation for thermal processes
- setting up the framework for the integration of the approach in an energy management system

In the next steps, the currently developed strategies will be transferred to other food production processes and other small and medium sized enterprises to verify both plausibility and applicability of the chosen approach. Apart from this, suitable optimization methods for the combination of batch and continuous processes have to be found.

The work is funded by Bayrisches Staatsministerium für Wissenschaft, Forschung und Kunst in the FORETA program.



# Green gasoline made from catalytic conversion of lignin

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Lignin, a three-dimensional, highly branched, and phenol based polymer structure with variously interlinked hydroxy- and methoxy-substituted phenylpropane units, in contrast, contains far less oxygen in the structure. A large quantity of phenolic compounds could be obtained, if suitable pyrolysis or hydrolysis techniques are applied. Quite high yields of phenolic oil (ca. 80 wt.%) have been reported in the patent literature via NaOH-catalyzed depolymerization of lignin in supercritical or near-critical water. This differs from most of the open literatures reporting that only about one fourth of lignin can be converted to phenolic products. We have recently explored a new route in depolymerization of lignin with combining base hydrolysis and protecting agents which can prevent the produced reactive substituted phenols to be polymerized. Additionally, new strategies using acidic hydrolysis/hydrogenolysis of lignin in presence of hydrogen have also been developed, which were also found to be efficient in cleaving C-O-C link bonds in lignin to obtain phenolic oil. However, due to the complexity of lignin structure, technology with sufficient efficiency and economic viability has not been realized on a large scale until now.

The currently most reported upgrading techniques of the depolymerized product use two approaches. One is based on zeolite catalysts at high temperatures (623

to 723 K) on which oxygenates are mostly converted to carbonaceous deposits and to a much lesser extent to alkanes. The other is based on hydrogenation and hydrodeoxygenation (HDO) with sulfide catalysts such as cobalt or nickel doped molybdenum sulfides.

For efficient conversion of phenolic compounds to hydrocarbons, two key problems have to be addressed. (1) Crude bio-oil contains approximately 15-30 wt. % water, which is difficult to be removed from the original solution, because the oxygen containing compounds easily oligomerize during the thermal separation. Therefore, bio-oil upgrading should be performed preferentially in the raw aqueous solution with water tolerant catalysts. Water as the main component of bio-oil is also proved to be an ideal medium for hydro-conversion of bio-derived phenols, polyols and terpenes. (2) Crude bio-oil contains large concentrations of reactive oxygen containing compounds, which are very unstable. Thus, bio-oil upgrading should be performed under mild conditions. Conceptually, the reductive step on hydrodeoxygenation of bio-oil in aqueous phase using dual functional catalysts (Pd/C with H<sub>3</sub>PO<sub>4</sub> or Raney Ni with Nafion/SiO<sub>2</sub>) under mild conditions (473 K to 523 K, 5 MPa H<sub>2</sub>) has been shown to be a very promising route.

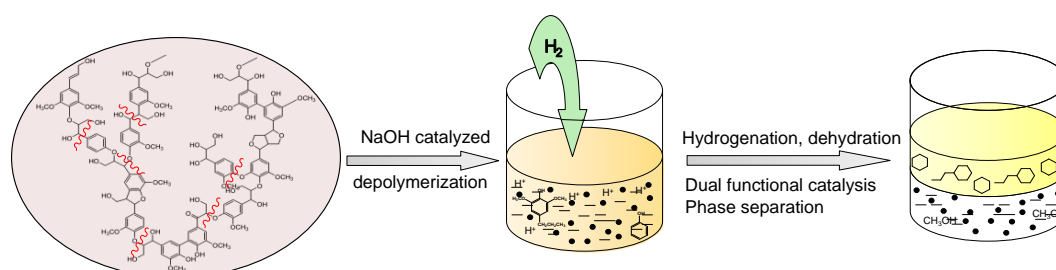


Figure 1. Combined cleavage of lignin and hydrodeoxygenation of phenolic oil to produce hydrocarbons.



# Morphology of bulk heterojunction systems for polymer-based photovoltaics

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Polymer-based photovoltaic systems are of very high interest for research groups as well as industry. The enormous potential of light weight and cheap applications supports the strong progress taking place. At present polymer-based systems already reached efficiencies of 8.5 %. Nevertheless, efficiency and lifetime of organic solar cells are still not high enough for a broad application.

A typical polymer based solar cell is a layered system containing blocking layers and the active layer between two electrodes. The active layer with a thickness of about 100 nm is normally a blend of two organic components, an electron donor and an electron acceptor, the so-called bulk heterojunction. Due to phase separation a nanostructured morphology by self-assembly processes is created in the active layer. In addition to the process condition during the solar preparation, especially post production steps like thermal annealing are used to control the structure formation. In summary, beside the electronic structure of the organic components also the morphology on several length scales is crucial for the photovoltaic performance.[1]

For the mesoscopic length scales one important parameter is the blending ratio of the used organic components in the active layer. We studied the influence of the blending ratio for polythiophene based systems on the nanostructure formation with grazing

incidence small angle scattering (GISAS). For all polymer systems a critical blending ratio with favorable minimal structures was predictable from theory.[2] The crystallinity of polymer chains is of utmost importance as it influences the absorption of the material as well as the charge carrier mobility. We investigated the influence of blending and thermal annealing on the crystal formation of a polythiophene based bulk heterojunction system. Grazing incidence wide-angle X-ray scattering (GIWAXS) is used to probe the crystallinity of thin films and to determine characteristic length scales of the crystalline structure. Moreover, the orientation of the crystalline parts regarding the substrate of both the homopolymer and the blended films is probed with GIWAXS. For the investigated system temperature annealing is found to improve the crystallization for both homopolymers. (Fig. 1) However, blending both polymers reduces or even suppresses the crystallization during spin coating as well as temperature annealing.[3]

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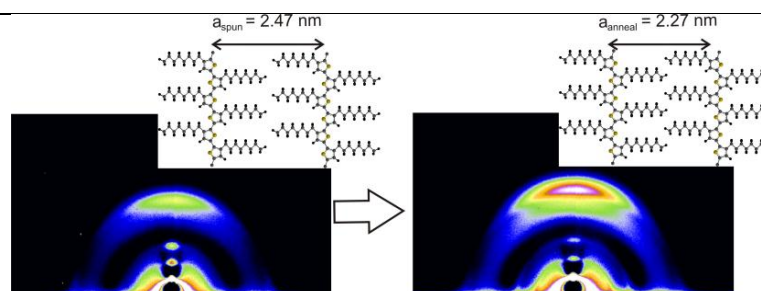


Fig. 1: GIWAXS pattern of thin as-spun and annealed P3OT films revealing crystal formation due to annealing.[3]

# Photovoltaics of nanoscale circuits comprising photosynthetic proteins

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The photosystem I (PS I) reaction center is a chlorophyll protein complex located in thylakoid membranes of chloroplasts and cyanobacteria. The photosystem I mediates a light-induced electron transfer through a serial of redox reactions. It is intriguing to incorporate the photosystem I into optoelectronic and photovoltaic nanoscale circuits, since the photosystem I exhibits outstanding optoelectronic properties found only in photosynthetic systems. The probability for absorbing a photon within the whole protein complex is determined to be close to 100 %, while the energy yield for the process is approximately 58 % [1]. The nanoscale dimension and the generation of 1 V photovoltage further make the PS I reaction center a promising unit for applications in molecular photovoltaic systems [2]. Utilizing a unique cysteine (Cys) mutation at the end of the photosystem I, we demonstrate how to incorporate the photosystem I into nanoscale electronic circuits [3]. The method allows studying nanoscale optoelectronic

and photovoltaic devices based on photosynthetic proteins [4,5].

We thank S. M. Kaniber, M. Brandstetter, L. Frolov, C. Carmeli, S. Richter, I. Carmeli, F.C. Simmel, D. Gerster, Hai Bi, J. Reichert, I. Visoly-Fisher, S. Sergani, and J.V. Barth for very fruitful collaborations. We further acknowledge financial support by the DFG via HO3324/2.

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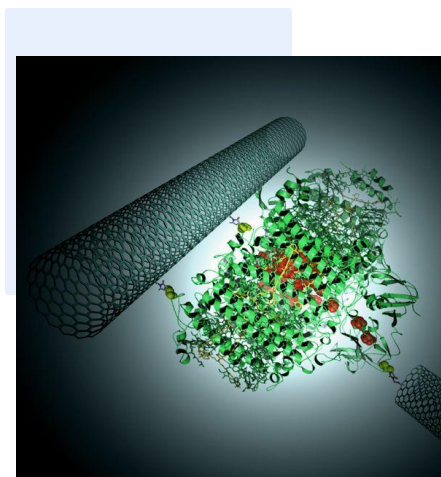


Figure: Single photosynthetic protein covalently bound to carbon nanotubes [3].

# Power Storage Requirements for Renewable Energies

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The worldwide demand for greenhouse gas reduction and reliable as well as sustainable energy supply promotes renewable energy technologies. A transition to renewable energy technologies is indispensable and future power generation will focus on wind, solar, biomass, and other alternative sources. For example, Germany will produce 50% of its power demand from renewable sources by 2030, and 80% by 2050, according to governmental energy strategy. However, a transition to renewable energy sources demands new power balance and control concepts. In contrast to conventional power plants, green energy sources like wind and solar are fluctuating and power production cannot be controlled directly. Today, wind produces by far more electricity than solar and current scenarios predict that wind will remain the most important renewable electricity source. In future energy systems wind will have to deliver electricity on demand. Either power storage systems or flexible power plants (coal, gas, biomass, solar) are needed that compensate wind fluctuations. The requirements and specifications of these systems are not known.

## Methodology and Results

Real wind power production data are available for Germany and Spain. Both countries are spatially distant within Europe, accounting for almost 60% of the total capacity installed in the EU-27. Data sets for all German transmission system operators and the Spanish grid are analyzed in intervals of 15 minutes over the time period of nearly one year. Average wind load factor and resulting storage level for Germany are shown in Fig. 1.

When assuming a controllable and steady power supply from wind (i.e. 4.2 GW base load), an ideal storage system will compensate for fluctuations. In high wind months (Nov/Dec/Mar) the storage is filled up to 4.8 TWh and cleared in the windless summer months (May-Aug). Considering spatial balancing effects, Europe needs a storage size of 8.3 TWh. Currently, the fluctuations are compensated by seasonal demand changes, and mainly by fossil power plants. However, the situation will impair as the wind capacity across Germany and Europe will increase. Therefore, the storage requirements are extrapolated to future energy scenarios. In 2030 the required storage capacity in Germany will be 9.4 TWh.

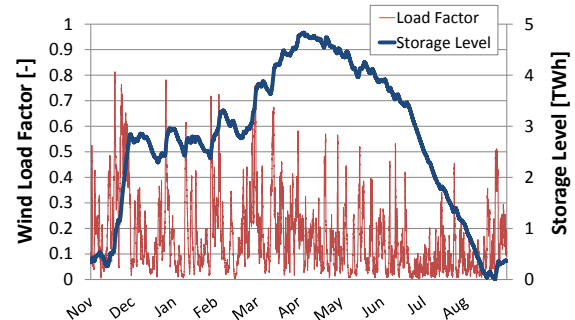


Figure 1: Wind data and calculated storage capacity to balance wind fluctuations for Germany 2009/10

In contrast, the German water pumped storage capacity is 0.04 TWh and a massive extension is not expected. Compressed air storage systems are a potential solution for short-term power compensation. As their storage capacity is low, they are not suitable for seasonal power balance. The implementation of water storage capacities in Scandinavia will require an enormous extension of the electricity grid that is hardly feasible due to resistance by local residents.

## New Storage Concepts

A new idea is the installation of power plants based on gasification. These are fuel (coal, biomass) flexible and are operated dynamically. Furthermore, the integration of a chemical storage and power overcapacities from renewable sources is feasible. A potential power plant concept is shown in Fig. 2.

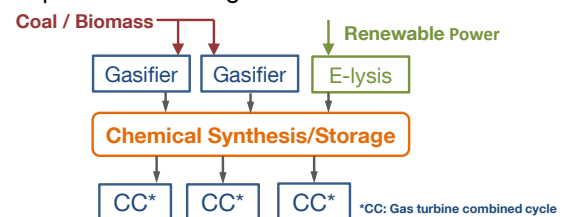


Figure 2: Future gasification concept

As energy is stored chemically (H<sub>2</sub>, CH<sub>4</sub>, Fischer-Tropsch fuel), storage dimensions are small and long term fluctuations of renewable power sources can be balanced. Power is produced in very efficient gas turbine combined cycles (CC) that adapt power output to current electricity demand. Different storage options are compared and discussed regarding their suitability to balance renewable energy sources.

# Storage of Bio-Energy – Substitute Natural Gas (SNG) as Contribution to Future Energy Systems

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Energy demand increases across the globe. Fossil fuels particularly crude oil, coal and natural gas are still the major sources of energy. Using biomass for energy production is an option which not only lowers the dependency on fossil fuels but also reduces CO<sub>2</sub> emissions.

Today biomass is converted to electricity by solid combustion in multi-megawatt power plants. An alternative solution for the distribution of bioenergy is the usage of the natural gas grid. Biomass can be converted to synthetic natural gas (SNG) via thermochemical gasification and a subsequent methanation process. After gas conditioning, the SNG can be fed to the existing natural gas grid. The overall conversion efficiency of such a process is supposed to be up to 80%. And the advantages are significant: Bioenergy in the form of SNG can be stored using the full developed natural gas storage technique and infrastructure which even today has a capacity of more than 200 TWh in Germany alone (most of it in underground gas storage facilities). SNG production offers several possibilities for further utilization and enlarges the application spectrum for biomass. Also it can act as temporary storage for fluctuating renewable energies like wind or solar. Figure 1 compares different storage options regarding capacity and discharge time.

SNG can be used for electricity production, heat production, as a transportation fuel and for domestic heating and cooking systems. In contrast to huge industrial scale plants of some 10-100 MWth, the SNG

production in small distributed systems is a way to minimize the local environmental impacts. A small scale process can be based on an indirect gasification such as for example the Biomass Heatpipe-Reformer® (BioHPR) developed at the Institute for Energy Systems. The objective of the work presented here is the investigation of an SNG solution for such small scale applications.

In contrast to natural gas, the biomass derived SNG (Bio-SNG) has a neutral or even negative CO<sub>2</sub> balance due to CO<sub>2</sub> capture and storage.

The process from biomass to SNG starts with the gasification of biomass which leads to a synthesis gas containing H<sub>2</sub>, CO<sub>2</sub>, CO, CH<sub>4</sub> and H<sub>2</sub>O mainly. This raw gas has to be cleaned from particles, tars, sulfur and chloride as well as some other contaminations. The subsequent main process step is the methanation, where H<sub>2</sub> and CO/CO<sub>2</sub> are converted to CH<sub>4</sub> and water. Residual CO<sub>2</sub> is removed and the water is condensed. For grid injection the SNG has to be pressurized finally. An exemplary overview of a schematic process chain is shown in Figure 2. Within the process chain to SNG there are still serious obstacles to handle as for example the tar problematic or the reactor design and cooling of the exothermic methanation reaction.

This overview wants to give a brief insight regarding the possible contribution of SNG to the challenging obstacles in future energy systems.

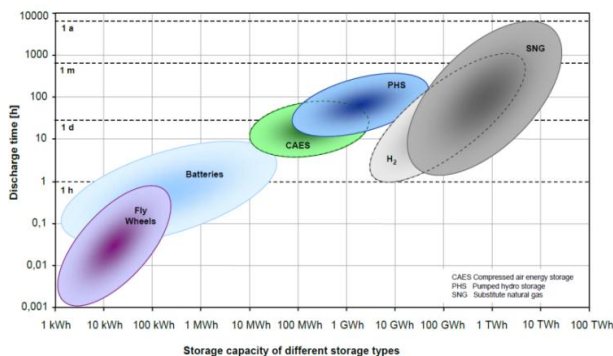


Figure 1: Energy storage options

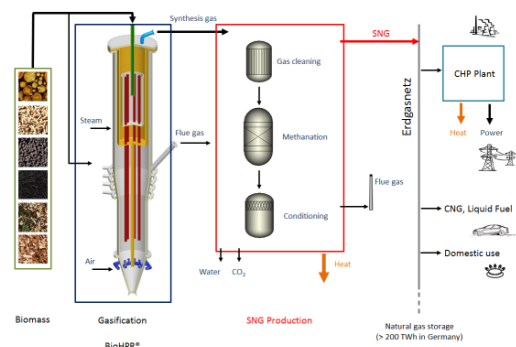


Figure 2: SNG process chain

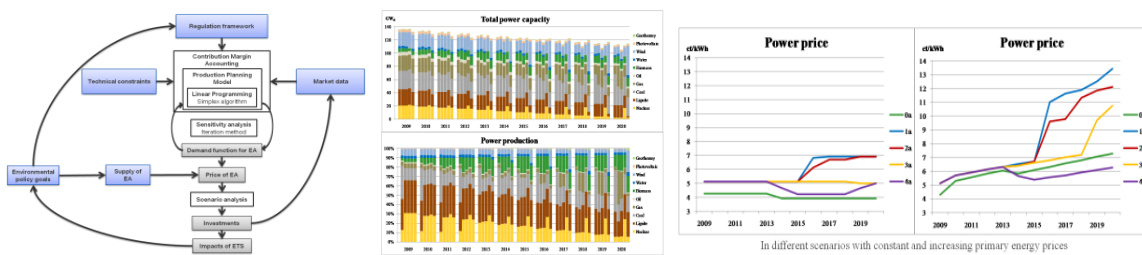
# Modeling long-term impacts of regulatory instruments on the German energy sector

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This study deals with regulatory instruments, but focuses especially on the Emission Trade System designed by the United Nations Framework Convention on Climate Change and introduced by the European Union in 2005. It is in our interest to forecast the effects of the European Emission Trade System on different indicators with economic importance (e.g. emission abatement, power price, import dependency, supply security, efficiency increase) and its costs up to the year 2020. Therefore we use an optimization model, in which

we consider the regulation framework, the market parameters and technical constraints for the German energy market as well as an endogenous price for emission allowances, running times of plants and capacity enlargements. After solving the model with linear programming in different scenarios we find, that the European Emission Trade System has strong impacts on production decisions, but low interest rates offered by the market incentive program are more effective in long-term decisions like plant investments.





## **4 Poster Presentations**

# Rotordynamic characteristics of brush seals for steam turbine application

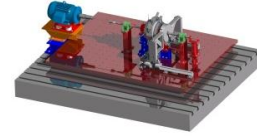
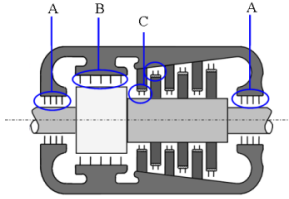
Manuel Gaszner

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A large part of the world's electrical energy supply is provided by power plants equipped with steam turbines. Rising requirements for better efficiency and a strict competition between Turbine manufacturers lead to higher power densities and challenging operation conditions. Leakage reduction is one of the most important aspects leading to efficiency improvement of turbomachinery. The most commonly used technology used at steam turbines to provide sealing at fixed and moving blades, diaphragm glands, piston and shaft ends is the labyrinth seal. To avoid rotor stator contact during operation, this seal type has to be designed with a minimum clearance what restricts the leakage performance. An alternative technology which is well known from gas turbines for aero-application, is the brush seal. Brush seals are dynamic sealing elements that have great potential as alternatives to conventional labyrinth seals in steam turbines. A brush seal consists of fine metallic or ceramic bristles closely packed into a seal housing consisting of front and backing plates. An angled arrangement of these bristles prevents them from buckling and allows the necessary bristle bending during rotor excursions. Brush seals can be designed as contact seals or with a small cold clearance depending on the application. The flexible nature of the bristle pack allows relative movement and vibrations of rotating and stationary parts during transient operation and the so called "blow down effect" caused by the lay angle and a radial pressure drop in the bristle pack enables the brush seal to close the gap between rotor and stator what leads to a further leakage reduction. This cannot be achieved with conventional labyrinth seals and makes brush seals very attractive in the market. Brush seals can be built into existing labyrinth seals replacing one or several seal fins, more axial place in the turbine is available that can be used to install more blade rows to increase the efficiency of the machine. The superior leakage performance of brush seals has already been proved but there is limited information on rotordynamic characteristics of brush seals. Several tests in laboratory scale showed that brush seals improve rotor stability in comparison with labyrinth seals but there are

different experiences with brush seals in steam turbine application. Thus there is need for detailed studies on destabilizing forces, stiffness and damping coefficients of brush seals. To realize and control the destabilising forces from brush seals and avoid stability problems of steam turbines in-service, a new project has been launched in collaboration with Technische Universität München supported by KW21 program. There are two test rigs at Institute of Energy Systems for studying brush seals at static and dynamic operating conditions. The static test rig allows to measure circumferential pressure distribution in seal cavities at different shaft eccentricity values, rotational speeds and inlet conditions. The term static stands for no shaft vibrations appearing during experiments because of the stiff rotor design. The calculation of static stiffness coefficients is based on integrating the circumferential pressure distribution measured in the seal cavities. The dynamic test rig allows identifying stiffness and damping coefficients by a whirling rotor system. The identification of the dynamic coefficients is based on the rotor excitation up to the stability limit using a magnetic actuator and on the effect of alternation of rotor vibrations due to aerodynamic forces acting in the seal. Both test rigs offer the flexibility of testing different sealing configurations assembled from a series of interchangeable rings. Parallel to experimental investigations on rotordynamic characteristics of brush seals, a theoretical method to predict stiffness and damping coefficients of brush seals will be developed. The method will be based on a full three-dimensional eccentric CFD model of the seal using the Reynolds-Averaged-Navier-Stokes analysis. The bristle pack of the brush seal will be modeled using the porous medium approach. This approach is computationally quite efficient and has proved suitable for leakage prediction. Part of this project is also to validate CFD tools for predicting seal leakage and rotordynamic performance. Lessons learned and derived guidelines will be documented, and exploitation of the results will be pursued.





# Electric energy generation by dynamic weight forces using the piezoelectric effect of PVDF

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Plane generator modules have been developed and successfully tested, which convert mechanical energy of dynamic weight forces into electrical energy. Mechanical energy, produced by walking or driving across the ground for instance, can be directly converted into electrical energy. The energy conversion is based on the longitudinal piezoelectric effect of mono-axial stretched PVDF-foil.

The fabrication of the generator modules was kept simple and inexpensive. Multilayer generator modules are built like wound capacitors. Thin commercial aluminum foils serve as electrodes. Two PVDF- and two Al-foils are stacked alternating above each other. This foil laminate was rolled in a desired diameter and flattened. Afterwards the flattened package was shrink-wrapped for conservation. As final production step a polarization process was carried out. High voltage was applied during this step at the electrodes. Thus, ferroelectric domains were aligned to get piezoelectric behavior of the PVDF-foil.

The design of the modules is characterized by a great flexibility in the geometrical dimensions. The dimensions of the modules were determined by the length and width of the foils and the roll diameter. Modules could be manufactured from small scale (e.g. 1cm<sup>2</sup>) to large scale (e.g. 800cm<sup>2</sup>) and with a varying number of layers in the package.

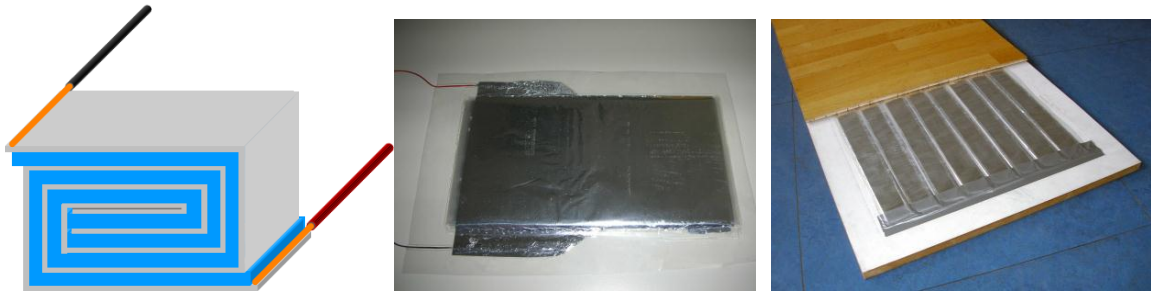
Generator modules were characterized with regard to the number of PVDF-layers in the pack, the geometrical dimensions and the weight force that affect them. Thus the electric energy output was measured at the electrodes during load cycles.

The electric energy generated increases with increasing mechanical load forces. Furthermore a rise of the energy output was observed with an increasing number of PVDF-layers.

Modules of 200cm<sup>2</sup> containing 56 layers PVDF loaded with weight-pulses of 70kg have generated about 2mWs/pulse.

In further experiments generator modules have been mounted under the parquet floor of an official building. This arrangement allowed the counting of persons going into and out of the building as well as generation of electricity. In these experiments an increase of electric energy generation with decreasing module size was observed.

The use of piezoelectric PVDF-foils appears to be more promising in comparison with similar solutions using piezoelectric ceramic substrates. PVDF is a flexible and very robust polymer material. It resists easily mechanical stress forces. In contradiction, ceramics are extremely brittle and require auxiliary protection in a harsh environment. With these properties PVDF generator modules offer a wide range of application in terms of sustainability. In crowded areas they could be placed on the ground and used as additional long-lasting and low-maintenance power supply for e.g. emergency lights, alarm systems, self-powered level-crossings, etc.



Figures: left: schematic of generator module, middle: laminated generator module, right: generator modules under parquet floor

# Waste heat recovery by means of ORC Orcan Energy – a TUM spin-off

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Sources of waste heat are widely characterized by a low temperature level. To recover the energy by means of a Rankine cycle, organic fluids show better performance and are more eligible than water due to a low boiling point. In the Organic Rankine Cycle (ORC) system the heat is used to evaporate a pressurized fluid which is expanded in a volumetric expansion machine that generates electric power. The low pressure vapor is condensed and recycled by means of a feed pump. The transferred heat in the condenser can be used for Combined Heat and Power applications.

The aim of the TUM Spin-Off Company Orcan Energy GmbH is the development of energy-cost efficient ORC systems for waste heat recovery with an electrical power lower than 50 Kilowatts.

Such system can be applied in different fields.

### Stationary Applications:

In stationary applications the system is used to increase the energy efficiency of various processes where heat is usually lost to the ambience. Suitable applications are:

- industrial processes (food, chemical industries)
- biogas engines
- solar systems

Typical temperature levels are in a range from 80 °C to 300 °C.

### Mobile Applications:

In mobile ORC applications the exhaust heat from combustion engines is used to generate mechanical or

electrical power that can serve as operating power for on board supply or hybrid driving systems.

A special challenge in mobile systems is the highly dynamic supply of waste heat. Therefore the dynamic operation of ORC system was tested and design strategy for optimized fuel saving was developed. It can be shown that fuel savings up to 10 % can be achieved in future systems.

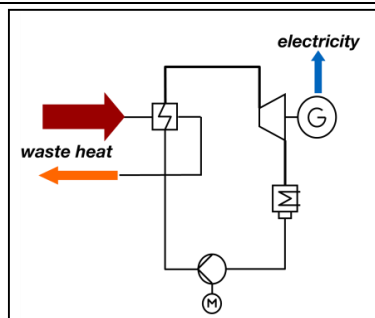
In current research the ORC system is further optimized in order to contribute to a sustainable and cost-effective power supply in the future.

### Working fields for students and graduates:

- Simulation of thermodynamic cycles
- Component testing
- Operation and testing of running systems
- Commissioning of new systems
- Product development
- Market research

### Acknowledgments:

The project ORCAN for setup of an ORC demonstration unit was funded by the Federal Ministry of Economics and Technology of Germany in order to enhance transfer of scientific results into spin off companies. Future research and product development is progressed by the spin-off company Orcan Energy GmbH.



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# Innovatives Biomasse-Pretreatment zur Biogasgewinnung

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Klimawandel, Verknappung fossiler Rohstoffe und die jüngsten Ereignisse in Japan haben insbesondere in der Bundesrepublik Deutschland zu einem Überdenken der Energiepolitik geführt. Der Konsens eine Energiewende einzuleiten zieht sich durch sämtliche politische Reihen. Das Reduzieren des Einsatzes fossiler Energieträger und der sukzessive Ausstieg aus der Atomkraft sollen durch erneuerbare Energiesysteme kompensiert werden.

Biomasse leistet dabei einen erheblichen Beitrag zur Grundlast in der Strom- und Wärmeversorgung. Der Biogastechnologie könnte hierbei eine Schlüsselrolle zukommen. Die Umsetzung von pflanzlicher Biomasse zu Biogas geschieht allerdings sehr langsam und unvollständig. Den prozentual größten Anteil der Trockenmasse von nachwachsenden Rohstoffen wie auch von Reststoffen stellt die dicht gepackte und damit widerstandsfähige Lignocellulose-Matrix, bestehend aus Cellulose, Hemicellulose, Lignin und Pektin, dar. Diese kann aufgrund deren struktureller Eigenschaften sowie natürlicher Grenzen der Mikrobiologie nicht hydrolysiert werden und verlässt den Biogasprozess weitestgehend ungenutzt. Darin enthaltene Zucker könnten ohne weiteres zu Biogas umgesetzt werden, vorausgesetzt die Substrate werden in einer bioverfügbaren Form der Mikrobiologie im Biogasfermenter bereitgestellt.

Angesichts der überwiegend dezentralen Biogaserzeugung auf meist landwirtschaftlichen Betrieben, werden bislang lediglich mechanische und biologische Aufbereitungstechniken in der Praxis eingesetzt. Speziell zur mechanischen Substrataufbereitung werden diverse Aufschlussverfahren zur Steigerung des Biogasertrages auf dem Markt angeboten. Außer einer Substratzerkleinerung werden dabei allerdings kaum Effekte zur Erhöhung der Bioverfügbarkeit hervorgerufen. Mit der bereits in der Papierindustrie bewährten Refiner-Technik kann eine optimiertere Biomasse-Desintegration bewerkstelligt werden. Infolge des Aufbruchs der Lignocellulose-Matrix werden durch begleitende Effekte die bisher unerreichbaren Fraktionen an Cellulose und Hemicellulose in eine bioverfügbare Form überführt.

Durch das in dieser Anwendung innovative Verfahren kann nicht nur eine Erhöhung der Biogasrate, sondern auch eine Steigerung des Biogasertrags von pflanzlicher Biomasse erzielt werden. Damit kann ein entscheidender Beitrag zum Umstieg auf erneuerbare Energiesysteme, insbesondere der energetischen Biomassennutzung, geleistet werden.

# Microbial Systems for Renewable Energy Supply from Biomass

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Plant biomass is a rich and renewable source of energy. Bacteria can be used in the process of energy production from this biomass in multiple steps of its utilization.

Plant cell walls are composed of several polysaccharides which are however difficult to hydrolyse. New cellulases and other depolymerases are necessary for production of the biofuels of the second and third generation.

Bacterial enzymes have evolved high efficiency of degradation. The most effective of their enzymes are organized in complexes which can be exploited for industrial production.

In a carbon-conscious world, energy production will be connected in a future biorefinery with production of platform chemicals through fermentation. Bioproduction (using microbial systems in biotechnology) avoids a number of problems occurring with other (e.g. thermo-chemical) ways of energy and chemical production. Only with biotechnology, sustainability is possible by

using all residues as fertilizer to replenish nutrients in the soil, including phosphorous, lignin and minerals.

The Department of Microbiology is engaged in research aimed at the use and improvement of microbial systems for the utilization of biomass for production of energy carriers and platform chemicals. This includes research in polysaccharide degradation for the production of sugars, both with whole cells (in vivo, e.g. in biogas plants) and with isolated enzymes and enzyme complexes (in vitro).

Genes from metagenomes and new bacteria with better traits are isolated (for new hydrolytic enzymes, fermentation products, or metabolic steps). Advanced screening systems for new enzymes are established. Selected bacteria are used for genetic optimization of product formation such as n-butanol, by metabolic engineering, transcriptome analysis, and test fermentations with the goal to investigate and to optimize the fermentation conditions or to utilize alternative substrates.

# Detection of Biogas Compounds Using Laser Induced Breakdown Spectroscopy and Raman Spectroscopy

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As a part of research and development of renewable energies fuel cells are getting important. Within a project funded by the European Union the use of biogas as energy source for high temperature fuel cells should be explored. Especially Molten Carbonate Fuel Cells (MCFC) are quite promising regarding their efficiency and environmental aspects. These cells gain energy by transformation of hydrogen which is produced by reformation of the main component of biogas methane. But the reactions on the anode and cathode of the fuel cells, which mainly influence the performance of the cell, are very sensitive to some compounds included in biogas depending on its source. Sulfur components, halogenated hydrocarbons and siloxanes impact the reactions in the cell and reduce efficiency and lifetime. Hence the cleaning of the biogas before using it for MCFCs and a continuous monitoring of the biogas composition are very important. The different aspects of the project like cleaning strategies, impact of compounds on cell performance and analysis of the biogas composition are handled by different groups. The Technical University of Munich is responsible for the detection of corrosive compounds in biogas. The requirements for the detection device are high since monitoring should be continuously to indentify problems in the cleaning and to avoid damages of the expensive fuel cells. Furthermore biogas can contain a wide range of substances which are harmful even in very low

concentrations. Regarding these aspects two analysis methods based on laser spectroscopy are chosen to develop a new analysis device.

The device is based on laser induced breakdown spectroscopy (LIBS) and on Raman spectroscopy. LIBS enables the detection of atoms by igniting a plasma. The light, which is emitted after the excitation with a laser, is atom specific, while the concentration is directly correlated with the intensity of the emission lines. In contrary Raman spectroscopy gives information about the molecular composition. A part of the light energy is transformed in molecular vibrations, while the rest is emitted as light. The energy difference between the excitation source and the emitted light is specific to molecules. To combine both methods an especial spectroscope is used, which has to different light entrances and thus can detect LIBS and Raman signals with the same device.

The big advantaged of the combination of LIBS and Raman spectroscopy is the possibility to get elemental and molecular information about the biogas sample with high temporal resolution. Furthermore both methods can be used in a wide range regarding the diversity of compounds and their varying concentrations.

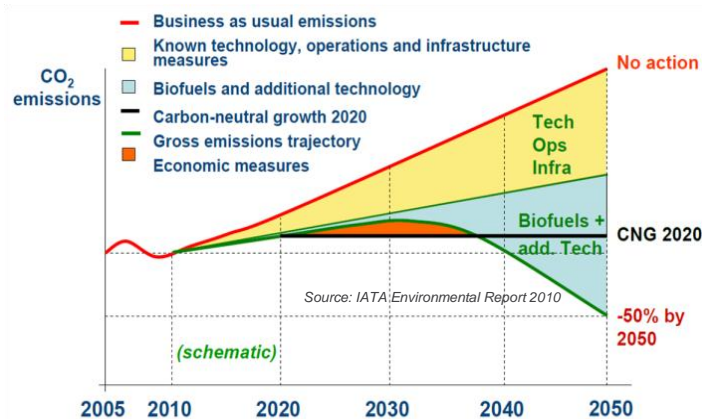
# Determining Sustainable Alternative Fuels for Aviation

Sonsoles Hernanz Albi<sup>a</sup>

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With all industries suffering the consequences of rising fuel prices and glimpsing the end of the oil era, focus is set on alternative energy sources. Aviation plays a key role in world social and economic development and its future growth requires sufficient fuel supply. The sustainability of this energy is of major importance for the sector due to the self-imposed emissions reduction targets for 2020 and 2050 (see figure below) to mitigate the impact on climate change and to the inclusion of aviation in the European Union Trading Scheme in 2012. Also, a secure supply of energy is urgently needed to avoid further complete dependence on oil and its price fluctuations. Technological improvements that lead to emissions reduction are based either on increasing fuel efficiency or on using alternative energy sources. However, with the expected traffic growth for the next 40 years, higher fuel efficiency cannot solely solve the problem. Alternative fuels can be classified into long-term technologies, such as hydrogen or fuel cells, and drop-in fuels, i.e. liquid fuels that can simply replace kerosene in current engines. Considering the technical challenges of hydrogen implementation, the limited storage capacity of batteries, and the long development times required in the aeronautical industry, drop-in fuels seem the best candidates to provide a secure alternative fuel supply in the medium-term. Drop-in fuels mainly comprise biofuels, gas-to-liquid, coal-to-liquid and waste-to-liquid technologies. Biofuels in particular

are the most promising to meet the sector's targets. The Lehrstuhl für Luftfahrtsysteme (TUM) is involved in the Lufthansa BurnFAIR Project, funded by the Bundesministerium für Wirtschaft und Technologie. For this project, Lufthansa will be using biofuel on regular flights for six months between Frankfurt and Hamburg, and the sustainability of the fuel will be evaluated. Setting the standards for the life-cycle analysis and the sustainability criteria of these fuels is currently a strong debate. Biofuels and other drop-in fuels not only introduce parameters regarding emissions, but also fresh water requirements, land use change, or the actual sustainability of aviation as an industry itself. These factors must be included when discussing future energy sources. Therefore, the answer for a sustainable and secure energy supply for aviation seems to lie in a combination of all these alternative fuels. None of them prove by themselves to be sustainable enough or producible in sufficient quantities to uniquely replace the expected oil demand by 2050. A well-planned and optimal share of different alternative fuels could be the path to achieve the goals for the sustainable development of aviation. However, uncertainties such as the deployment of these technologies or potentially harmful drivers of climate change other than greenhouse gas emissions must still be addressed.





# Statistical modeling of high frequency turbulence

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Wind energy is nowadays one of the most popular sources of renewal energy. The main resource, the wind speed, is characterized by fully developed turbulence, analyzed by Kolmogorov in his celebrated series of papers that spans from 1941 to 1963.

Therefore it is important to understand and to model the behaviour of the wind resource, in order to achieve a better windfarm design.

We base our stochastic turbulence modelling on Barndorff-Nielsen and Schimegel

(<http://dx.doi.org/10.1137/S0040585X9798316X>) that gives an intuitive but flexible modellistic approach to turbulence and finance. Moreover, it is also easy to simulate.

Its main ingredients are a kernel function, which models the memory of the system, and

a driving stochastic intermittency process, which represent the instantaneous energy dissipation or the volatility.

We suggest an estimator for the kernel function, whose prior knowledge is the used to recovery the intermittency process. We apply this statistical estimation method to high frequency turbulence data (sampled at 5000 Hz).

This framework includes as a special case the flexible class of continuous time ARMA processes.

This is joint work with Peter Brockwell (Colorado State and ColumbiaUniversity) and Claudia Klüppelberg (Technische Universität München)

# Efficient Methanol Synthesis Catalysts Long-Term Stability and Modelling of Deactivation

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Methanol is with a production volume of 47 million tons per year one of the most important base chemicals. A large part of the alcohol is used as a C1 building block in chemical production and converted into formaldehyde or acetic acid. Furthermore, it can be used directly as fuel or transformed into hydrocarbons using the MTO-Process. Used in a Direct Methanol Fuel Cell (DMFC) it becomes increasingly important as a mobile and clean source for electric energy.

Due to the fact, that methanol is liquid at room temperature (b.p. 64.7 °C), there are some benefits compared to gaseous energy carriers: There is no need for a complex and expensive storage device like for hydrogen and because of the absence of increased storage pressures the systems are safer. These advantages led to the claim of the so called "Methanol Economy" as a long-term sustainable solution for the fossil energy problem [1]. In order to support current research and development in this field, a cheap way to produce methanol is essential. Therefore, efforts have to be made in the research of new, sustainable ways to produce methanol (e.g. direct reduction of CO<sub>2</sub>) as well as in improving conventional processes for the methanol synthesis using synthesis gas.

The catalysts used in the industrial production of methanol are ternary Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> systems. These are rather cheap, nontoxic and display good activity. However, the systems rapidly deactivate in the first few hundred hours (formation period) and then reach a quasi stationary state which is accompanied by slow deactivation (steady-state deactivation). One of the most accepted reasons for the deactivation is the agglomeration of the dispersed active copper particles. A detailed mechanism or at least a reliable description of the deactivation kinetics is not yet known. Unfortunately, there are also no long-term studies of this process available in literature, which makes it impossible to systematically study this phenomenon. The aim of this project is the measurement and characterization of different deactivation factors, as well as the mathematical description of the deactivation kinetics.

Due to the fact, that the steady-state deactivation is a slow process, the concept of "Rapid-Aging" is applied. Here selected catalysts are stressed in long-term experiments (about 1000 hours) under controlled conditions, specifically high temperatures up to 250 °C and high partial pressures of water, methanol and carbon monoxide. The activity of the catalysts is evaluated periodically using kinetic experiments. In order to fulfill these requirements, a setup for kinetic experiments was built.

The setup consists of four parallel reactors that can be heated up to 350 °C. Analysis is performed by gas chromatography. The whole system is suited for pressures up to 65 bar and the reactors can be removed for further analysis without contaminating the catalyst with air. Using a mass spectrometer the free copper surface area can be determined by frontal chromatography without removing the reactors. The automated process can run more than 1000 hours without interruption. By varying temperature, synthesis gas composition or catalyst specific parameters a systematic study of the process parameters on catalyst deactivation can be accomplished.

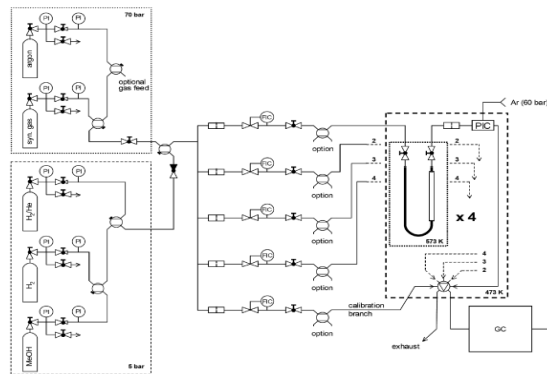
The deactivation will be modelled using a modified general power law model. This provides the possibility to describe thermal deactivation factors as well as specific influences of the gas atmosphere composition [2].

The kinetics of selected catalysts will be evaluated using Langmuir-Hinshelwood-Hougen-Watson models [3]. In combination with the measured copper surface area and time dependent activity these models will be extended with a deactivation term. This more detailed kinetic information is important for the modelling of macrokinetic limitations, which is another possible reason for the catalyst deactivation and also an important issue in industrial catalyst design.

The obtained data may lead to a better understanding of a possible catalyst deactivation mechanism which is essential for the systematical improvement of the catalyst's long-term stability.

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# Ethene-to-Propene-Reaction on Supported Nickel Catalysts

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Propene is after ethene the second most important basic organic chemical. The demand of propene is constantly increasing due to the growing need of polypropylene and propylene oxide. Mostly, propene is obtained as byproduct during steam cracking of naphtha to ethylene and catalytic cracking of crude oil into petroleum fractions in refineries. To a minor degree propene is synthesized via metathesis of ethene and butene to propene known as ABB Lummus process and the dehydrogenation of propane (Fischer-Tropsch synthesis). A more sustainable route for the production of propene is the conversion of biomass to propene over ethanol and ethene as intermediates. The challenging step in this connection is the ethene-to-propene-reaction. For this process heterogeneous catalysts consisting of nickel supported on mesoporous silica are interesting like Nickel-MCM-41 reported by Iwamoto et al [1].

As supporting material mesoporous silica – SBA-15, MCM-41 and MCM-48 [2] – was applied and coated with nickel via incipient wetness impregnation. As nickel precursors nickel nitrate and nickel citrate were used. Furthermore, uncalcined MCM-48 was template ion exchanged [1] with differently concentrated nickel nitrate solutions. The nickel content was in the range of 0.5 to 9.0 wt%. The characterization of these catalysts was carried out by physisorption, thermogravimetry, XRD and ICP-OES.

The catalytic activity of the as-synthesized catalysts was tested in a fixed-bed reactor at reaction temperatures between 300 and 400°C. The gas flow was composed of

helium and ethene (2-10 %). The product gas flow was analyzed on-line with a gas chromatograph.

Nickel supported on mesoporous silica shows high selectivity to propene. As by-products mostly butenes (1-butene, cis- and trans-butene) can be observed, which reflect the presumed reaction mechanism (Figure 1).

Deactivation of all catalysts occurred without the supply of water vapor within a few hours. If the educt gas flow contains a small amount of water vapor, the ethene-to-propene reaction can be operated several days with only a minor reduction of catalytic activity. All catalysts could be completely regenerated in synthetic air at 500°C. The impregnated catalysts performed slightly different to the template ion exchanged catalysts.

## Impregnated catalysts (IMP)

Conversion of ethene and yield of propene decreased in the order Ni/MCM-48 > Ni/SBA-15 > Ni/MCM-41. In comparison to nickel nitrate smaller and well dispersed nickel oxide particles on the support were formed with nickel citrate [3]. Best results were obtained with low nickel loading (~1 wt% Ni) and high nickel dispersion. Nickel contents higher than ~2 wt% and the addition of water vapor resulted in the production of methane as main product and only marginal amounts of propene.

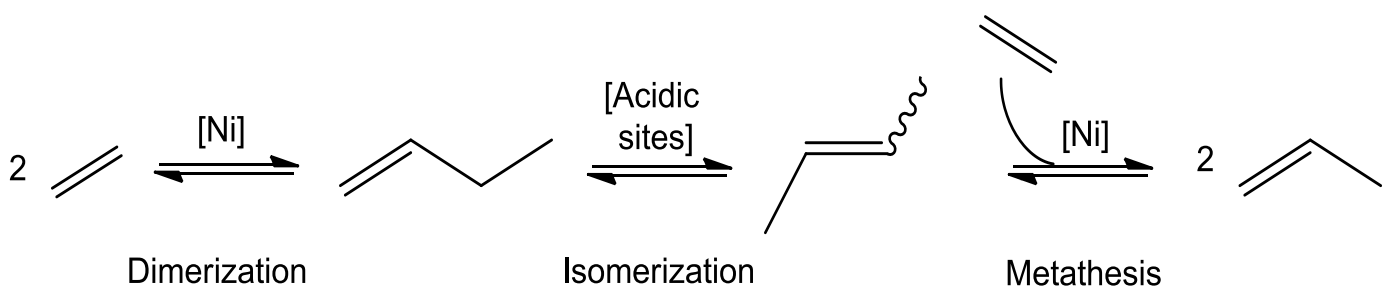
Template ion exchanged catalysts (TIE)

The nickel content of the template ion exchanged catalysts was in the range of 5 to 9 wt% Ni. Fortunately, addition of water vapor did not change the product spectrum of these catalytic systems and only traces of methane were produced. Ivory-colored catalysts were much more active compared to brown ones (indicating bigger nickel oxide particles) with the same nickel loading. The slightly different catalytic behavior of TIE- to the IMP-materials can also be explained with the appearance of dissimilar reflexes in the XRD-diffractograms.

These catalysts were also active in the direct conversion of ethanol to propene. Complete dehydration of ethanol to ethene was observed, which opens a new field of application for nickel supported on different mesoporous silica.

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[1].Figure 1: Presumed reaction mechanism for the ethene-to-propene reaction

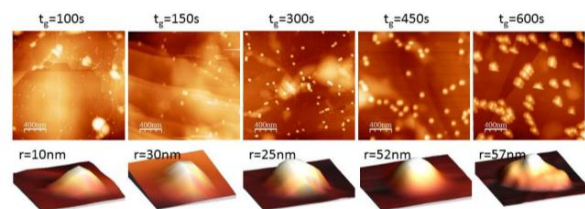
# Size-dependent activity of metal nanoparticles: Electrochemical preparation and investigation of nanostructured catalysts on planar carbon surfaces

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The properties of nanoparticles often show considerable differences as compared to bulk materials. The understanding of this change in properties with morphology is crucial for the design of effective catalysts for use e.g. in fuel cells and batteries. Platinum is the most widely used catalyst material, in technical catalysts it is usually found in the form of nanoparticles supported on carbon. While Platinum is an active material in its bulk and its nanostructured form, the nanoparticles are used to achieve an optimized surface/material ratio. Mono- and submonolayers on Au(111) surfaces showed an tremendous increase in activity regarding the hydrogen evolution and oxidation reaction (HER and HOR). This was ascribed to an interaction of the nanoparticles with the support. In contrast to platinum, gold in its bulk form is usually behaving as an inert material in acidic solutions. However, results on supported gold nanoparticles exhibit an enhanced catalytic activity regarding different reactions (such as CO and H<sub>2</sub> oxidation in heterogeneous catalysis and oxygen reduction in electrocatalysis) for small particle sizes. The origin of this enhancement is still not fully understood. A change in electronic properties due to different particle sizes, which are particularly relevant for particles with size of a few nanometers, might influence the catalytic activity of the particles. Also the support material might have a major influence on these small particles. We aim at a better understanding of the size-dependent catalytic activity by the investigation of platinum and gold nanoparticles on planar carbon substrates. In the case of highly oriented pyrolytic graphite (HOPG), the special layer structure results in a very weak binding of metal particles on the HOPG basal plane. In the case of diamond, the particles are more strongly bound to the

surface. However, the growth proceeds three-dimensional, and the influence of the substrate should be small. Therefore, the activity of the metal nanoparticles should be influenced mainly by particle size for both substrates, but maybe partly also by particle-substrate interaction in the case of diamond. The particles were prepared by electrochemical reduction of different metal complexes using a potentiostatic double pulse method. In a first step, nuclei are formed on the support. This is achieved by applying a short, high overpotential potentiostatic pulse. In a second step, these nuclei grow slowly to their final size, while no further nucleation takes place. This is accomplished by applying a low overpotential for various times. By varying parameters such as the potentials and deposition times of the double pulse, the particle density and particle size can be controlled. We varied only the duration of the second pulse  $t_g$  and therefore achieved surfaces with a constant particle density and different particle sizes. These surfaces were used to investigate the size-dependent electrochemical activity regarding different reactions. While the platinum and gold particles didn't show a size effect for the hydrogen related reactions HER and HOR, the ORR on gold nanoparticles shows an increased activity for decreasing particle size.



Pt nanoparticles on HOPG: for a variation of particle sizes the growth pulses with different durations  $t_g$  were applied

# Nanotubular TiO<sub>2</sub> – interdependence of Titanium grain structure and tube morphology

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Self-organized nanostructured oxides grown by optimized metal anodization have attracted remarkable interest in the past decades. Starting with the growth of nanoporous alumina [1], this type of anodic oxide films can nowadays be grown on various valve metals and their alloys using dilute fluoride based electrolytes. Upon all valve metal oxides, nanotubular TiO<sub>2</sub> on Ti [2,3] is among the most promising structures since it offers several interesting functional properties.

The growth of self-organized TiO<sub>2</sub> nanotube arrays on electropolished and non - electropolished Ti sheets was investigated for two different electrolytes, being a fluoride ion containing phosphate buffer as well as a glycerol-based electrolyte. A systematic structural and morphological characterization was performed revealing an interdependence of the crystallographic orientation of the grains in polycrystalline Ti and the growth rates and properties of nanotubular TiO<sub>2</sub> layers.

On non-electropolished Ti substrates, no grains are visible. No real influence of the crystallographic structure on the growth rate is visible and the tubes have the same medium length of ~3.0 μm all over the surface. Their length depends on the fluoride

concentration of the electrolyte and on the anodization time.

On electropolished substrates a well defined grain structure is visible and a strong influence of the crystallographic orientation on the growth rate of the tubes can be observed. At least 4 different zones with nanotubes of different growth rates can be found. The nanotube length varies from ~ 1.1 μm to ~ 3.2 μm.

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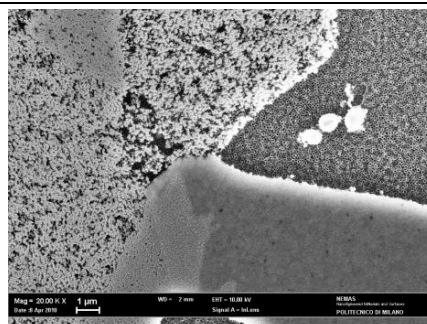


Fig. 1: TiO<sub>2</sub> nanotube growth depends on the grain structure.

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# Multiscale modeling for green engineering: Differently detailed models to describe methanol synthesis over a ternary copper catalyst

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## Introduction

Methanol counts among the most important basic chemicals in industry and becomes more and more important as a chemical energy carrier, but can also be used as fuel for fuel cells. Moreover it is a promising hydrogen storage, which can be handled by the existing gasoline infrastructure. Methanol is commercially synthesized over Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts. Depending on the level of understanding for the catalytic reaction different approaches in engineering multiscale modeling can be applied. Global kinetic models, i.e. in the simplest case power laws or Langmuir-Hinshelwood-Hougen-Watson models (LHHW), are mainly used for reactor design and operation of chemical reactors. Modeling on a microkinetic level includes all elementary steps on the copper active sites. This work compares three approaches to model the methanol synthesis under industrial conditions with respect to their applicability and validity.

## Experimental

The modeling is performed on the basis of kinetic measurements in a laboratory scale single-stream fixed-bed reactor. Experimental conditions range from 5 to 60 bar and 463 to 523 K, also varying the composition of the dry synthesis gas. Hereby diffusion and mass transport limitations can be avoided. In a good approximation the fixed-bed reactor is modeled as an ideal plug flow reactor. Experimental data were also taken from temperature-programmed flow experiments in order to constrain further the microkinetics. Thorough parameter estimations have been performed based on the experimental data.

## Results/Discussion

The power law gives information on the reaction order of each component; however, it is not very precise in predicting the measured carbon conversion. In contrast to that, the LHHW model can predict the rate of methanol formation in a satisfying way. The implementation of an adsorption term, which depends on pressure and temperature, clearly enhances the quality of the model. Figure 1 shows a parity plot of the measured compared to the calculated carbon conversion. Recent works show that ternary copper catalysts underlay morphology changes depending on the gas atmosphere [1, 2]. This was also referred as wetting/non-wetting behavior [3]. Reducing gases like hydrogen or carbon monoxide can create oxygen vacancies in the Cu-O-Zn interface. The microkinetic model by Ovesen et al. [4], which incorporates such morphology changes, is implemented and adapted in order to investigate different aspects in methanol synthesis. Thereby, differences in the exposed copper low index planes (111/110/100) have been considered [4]. A sensitivity analysis for typical methanol synthesis conditions showed that the most influencing parameter on the catalysts morphology in such a model is the amount of water produced in the reaction. It strongly influences the catalyst's performance and the morphological changes of the catalyst. In a next step, the microkinetic model can be used to describe the catalysts deactivation behavior when reducing or oxidizing components such as carbon monoxide and water adsorb on the surface and change the morphology of the catalyst and therefore its activity. This is a new way to describe deactivation of the catalyst in contrast to typical power law deactivation models [5].

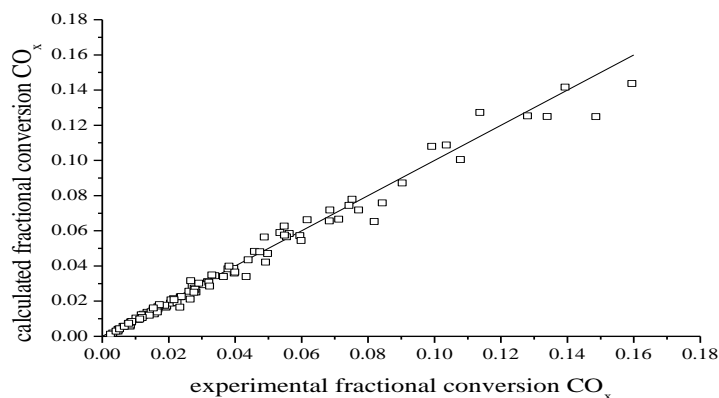
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# Study of enzymes tethered to Au(111) surfaces

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In fuel cell systems and metal-air batteries, the oxygen reduction reaction (ORR) at the cathode side is still one of the performance-limiting factors. Extensive efforts are made to improve existing catalysts and to find new materials with lower overpotentials for oxygen reduction in order to improve its sluggish kinetics.

Enzymes like laccase are ideal candidates for the investigation of the oxygen reduction reaction due to their high redox potentials and their high catalytic activity towards the ORR. In this work, laccase molecules are immobilized on Au(111) surfaces to be studied by electrochemical methods and scanning probe techniques.

One challenging task is tethering the enzymes onto the Au(111) surface without destroying their tertiary structure in order to preserve the activity of the molecules. Thiols are attached to the gold surface via self assembly to establish an interface between the highly charged Au(111) surface and the organic molecules. The immobilization of laccase molecules has to be achieved via conductive linkers that are placed inside the thiol self-assembled monolayer (SAM) and that are covalently bound to the gold and to the enzymes to obtain direct electron transfer between enzyme and electrode. Adjusting these linkers to the enzyme structure is necessary to guarantee a proper

enzyme orientation and to enable a transport of the electrons to the enzyme redox center.[1,2]

The surface coverage and surface pressure after functionalization with thiols and enzymes are determined using electrochemical methods like cyclovoltammetry, capacity measurements and chronocoulometry. The absolute values of surface capacity and resistance are determined with Electrochemical Impedance Spectroscopy (EIS). The electrocatalytic activity of the tethered enzymes is studied using cyclovoltammetry.

In-situ scanning probe techniques like electrochemical scanning tunnelling microscopy (EC-STM) and scanning electrochemical potential microscopy (SECPM) are used to determine enzyme coverage and orientation. Particularly SECPM provides the unique ability of contactless probing of non-conductive surfaces or surfaces with low conductivity, thus allowing imaging of sensitive molecules such as enzymes.[3]

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# TiO<sub>x</sub>C<sub>y</sub> based supports for application in electrocatalysis

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Carbon based materials are often used as supports in real catalyst systems, but have the disadvantage to be prone to corrosion which can cause dissolution and catalyst agglomeration. Oxide supports are more stable and promising for medium and high temperature applications.

TiO<sub>2</sub> has a wide field of applications that are based on its semiconductive nature, for example in photocatalysis or dye-sensitized solar cells. Reduced titania has shown to be a suitable support for Au nanoparticles that exhibit activity for CO oxidation in UHV catalysis [1].

To expand the utilization of TiO<sub>2</sub> to applications that require a fast electron transport in corrosive environments, such as functional electrodes in batteries or electrocatalyst supports in fuel cells, the material has to be made conductive and inert towards reoxidation. This can be achieved by employing a carbo-thermal reduction treatment converting the TiO<sub>2</sub> into a Magnéli-like oxy carbide compound (TiO<sub>x</sub>C<sub>y</sub>) that shows stable semimetallic conductivity. As found for nano-tubular TiO<sub>2</sub>, the converted electrodes have a substantial overpotential for O<sub>2</sub> evolution and provide an efficient support for electrocatalytic methanol oxidation [2].

Model systems consisting of electrocatalytically active metals like Pt, Pd or Au, deposited on compact, flat

TiO<sub>x</sub>C<sub>y</sub> substrates are being developed and investigated in terms of their electrocatalytic activity for CO and alcohol oxidation. A parameter study has been performed for compact TiO<sub>2</sub> films on Ti sheets to investigate and optimize the carbo-thermal reduction process. The composition and morphology of the films before and after the conversion have been studied with XPS, SEM and AFM. The electronic properties and the stability were investigated electrochemically.

To test the applicability of compact TiO<sub>x</sub>C<sub>y</sub> as support material for electro-catalysts, a Pt deposition study was performed using an aerosol assisted deposition (AAD) technique [3]. The Pt covered substrates were then investigated in terms of their performance for methanol and ethanol oxidation.

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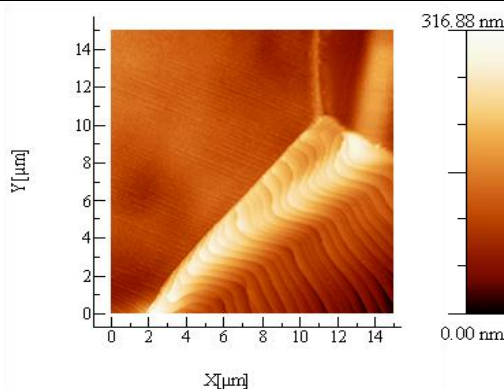


Figure 1: AFM micrograph of an anodic compact oxide film after carbothermal reduction.

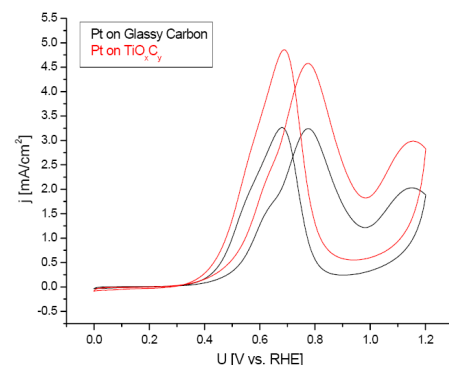


Figure 2: Ethanol oxidation reaction on Pt, deposited by AAD on a Glassy Carbon and on a TiO<sub>x</sub>C<sub>y</sub> substrate, in 0.5 M EtOH in 0.1 M HClO<sub>4</sub> with a scan rate of 10 mV/s.

# Structured polymer films and their application for organic photovoltaics

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Due to the increasing worldwide consumer demand on power, new and especially environmentally friendly ways for electricity power generation have to be explored. Photovoltaics have therefore proven to be a practical candidate to locally produce electricity at acceptable costs. The increasing market demand, also supported by governmental benefits, already led to the fabrication of efficient large scale solar cells based on silicon. Nevertheless a minimum operating time of over two years is required to reach a positive energy balance of such silicon solar cells, which require high energetic fabrication steps. Therefore organic solar cells (OSC) are very promising candidates which combine low production costs with other design opportunities such as mechanical flexibility and ultra-thin solar cell properties.

Up to now organic solar cells based on poly(3-hexylthiophene) (P3HT) and the fullerene derivate [6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM) have already reached power conversion efficiencies of up to 5% [1]. Therefore this polymer:fullerene-system is very well studied and helped to understand the fundamental physics behind the charge carrier generation and separation in conducting polymer blend films. Nevertheless the efficiencies of OSCs have to be improved in order to compete with their inorganic counterparts. Na et al. have recently shown that the performance of P3HT:PCBM solar cells can be improved by almost 20% due to an additional surface structure of the active polymer layer [2]. Here we

present a novel structuring approach which can be used to texture PEDOT:PSS films, which are commonly used as underlying electron blocking layers for organic solar cells. For this method the aqueous polymer solution is doped with glycerine and structured with a channel shaped PDMS stamp at elevated temperatures and constant pressure. Figure 1(left) shows a topographic atomic force microscopy image of such a structured PEDOT:PSS film. The surface properties can be tuned via the glycerin concentration, which softens the polymer film, and the experimental parameters during the imprinting. Afterwards the structured PEDOT:PSS film is covered with the active P3HT:PCBM layer and aluminum contacts are evaporated on top. Figure 1(middle) shows an image of such a final device including its grating structure, which leads to the generation of a rainbow spectrum under an inclined angle of observation. The gain in efficiency can be seen from the corresponding current-voltage curve (IU-curve) in Figure 1(right). The structured solar cells have an enhanced current generation of 24% leading to an improved overall efficiency of 20%. In this work different structure morphologies and their influence on the solar cell performance are discussed.

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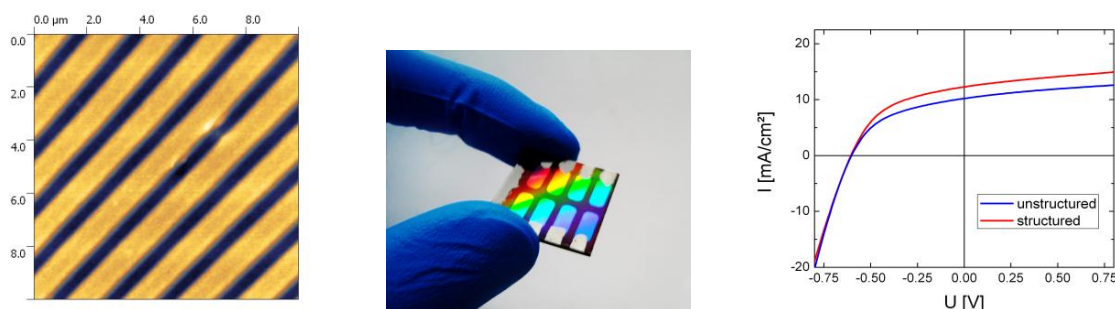


Fig. 1: (left to right) Superstructured PEDOT:PSS film as probed with AFM, final device including grating structure and corresponding IU curve.

# Solvent induced morphology in polymer-based organic photovoltaics

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The steadily increasing world wide energy consumption forces additional sources of energy for future. Green renewable energy sources seem quite attractive in this perspective. Among all the possible renewable energy sources, solar energy is one of the most promising candidates due to its unique properties. Polymer-based solar cells, as a young branch of photovoltaics, have attracted tremendous interests due to low production cost, mechanical flexibility, light-weight property, and similar theoretical power conversion efficiency (PCE) as compared with silicon-based solar cells (around 16%) [1].

Relatively high performance polymer bulk heterojunction (BHJ) solar cells (Fig. 1), based on self-assembly phase separation of an electron-donating conjugated polymer P3HT (region-regular poly(3-hexythiophene)) and an electron-accepting fullerene PCBM (phenyl-C61-butyric acid methyl ester), have become of great interest for the application of organic photovoltaics. Although the PCE of polymer solution-based solar cells have been improved up to 8% [2], the in-depth investigation of the three-dimensional (3D) morphology is crucial for a fundamental understanding. For example the influence of different solvents on the morphology is still not fully

understood, although it's well known that the solvent properties strongly influence the morphology formation of the film, which directly determines the final PCE.

In this work, we focus on the impact of the used solvent on the morphology of the active layer. The surface structure is investigated by optical microscopy and AFM. In combination with scattering techniques such as XRR, GISAXS and GIWAXS, revealing the inner structure as well as crystallinity, the whole morphology of the active layer is detected, and the representative vertical composition is shown in Fig. 2. Consequently, the different morphologies formed from different solvents are determined and compared with the corresponding performance of the systems. [3]

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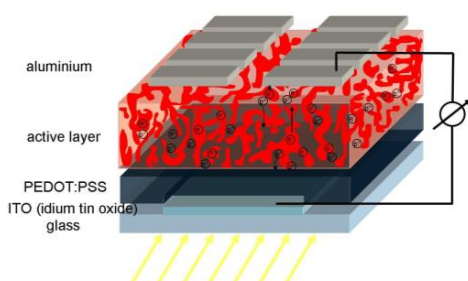


Fig. 1:  
Sketch of layered device structure of a typical BHJ solar cell

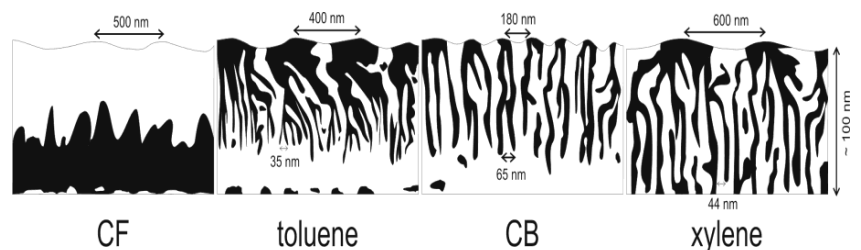


Fig. 2:  
Reconstructed schematic morphologies of annealed P3HT:PCBM films made from chloroform, toluene, chlorobenzene, and xylene solutions. [3]

# Organic photovoltaic: Three component systems

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Today, most people associate the expression photovoltaics with silicon based solar cells. The reason being that over recent years photovoltaic installations on rooftops and elsewhere strongly emerged and harvested, for example, 6.2 TWh in Germany in 2009 [1]. However, despite its strong position on the market, an intrinsic problem of silicon-based solar cells is the need to produce material of very high purity. This results in high energy and monetary cost during production. A novel approach is to use organic photovoltaic systems. In contrast to silicon based solar cells, organic photovoltaic does not require highly purified silicon because it uses a different type of semiconductor, so called organic semiconductors. The discovery of these organic semiconductors, also known as conducting plastics, was rewarded with the Nobel Prize in 2000. Organic semiconductors are of major interest these days because they are promising major simplifications in production: organic substances can be solution processed, resulting in extremely simplified and therefore cost efficient production methods. Furthermore there will be hardly any limitations on shape and form. There are even approaches to allow bending of the organic solar cells. If this technique matures this will allow a totally different approach to harvest solar energy than what we know of today.

However, efficiencies of organic photovoltaic devices are still not comparable with their silicon-based counterparts. Although steadily increasing over the last years, the reached efficiencies are more than a factor of 3 below those that can be achieved with silicon

technology. One reason is the still very limited fundamental understanding of the underlying processes in organic photovoltaic systems. To obtain efficiencies with organic photovoltaic systems that are interesting for industrial applications more work is needed.

One key issue is the extremely short photon conversion length, called exciton diffusion length, in organic semiconductor based cells. Excitons created by the incoming light need to be split in separated charges within a few tens of nanometers to harvest energy. Therefore the morphology of such systems is extremely important [2]. To understand the implications of the internal structure and its formation process of the solar cells, different optical and structural methods are used.

So far binary systems have typically been used in organic photovoltaics [2] where a p- and an n-conducting polymer are in close contact. The addition of a third component to modify the morphology of these binary systems is an interesting and promising approach. In this work we focus on the influence of such a third component on a standard two-component system. The aim is to improve organic solar cell efficiencies and understand the reasons for it, such that this can be exploited to shape innovations in the renewable energy usage of the future.

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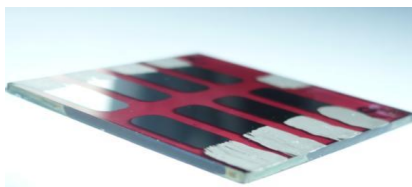
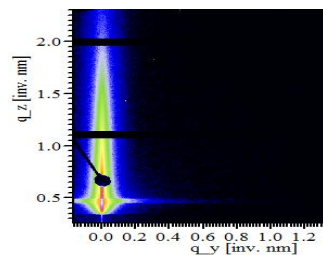


Fig. 1: example of test solar cell during experimental research



Grazing Incidence X-ray scattering image, a technique used to examine the internal structure of organic photovoltaic systems

# Investigation of the morphology of photoactive polymer layers for flexible solar cells

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Recently, the interest in photoactive polymer films in organic photovoltaics increased dramatically because of their promising application in touch screens, LCDs, OLEDs and solar cells. [1-2] Compared with conventional inorganic photoactive thin films, polymer films have many unique features such as mechanical stability, light weight and low cost.

There have been already many studies on organic solar cells, but only little attention has been focused on fully flexible organic solar cells so far. Carbon nanotubes (CNT) are among the most promising candidates of flexible electrode materials, which can be deposited on flexible PET substrates instead of normally used glass substrates. Compared with the traditional rigid ITO electrodes, CNT film electrodes have many unique properties such as good flexible mechanical properties, high work function, low cost and sufficient quantity of carbon. As a consequence, flexible solar cells and panels will be applied in future for many kinds of products to be introduced into the market including solar backpacks, solar thin film clothing and athletic apparel.

The properties of the electrodes such as transmission, and sheet resistance are crucial for solar cells. So we first investigated these properties of ITO on glass, ITO on PET and CNT on PET. The PET substrates exhibit less transmission in comparison with the conventional glass substrates. Compared with ITO electrodes, CNT

electrodes have in addition a slightly lower transmission in the wavelength range of 400 nm to 1100 nm, while CNT has a broader transmission than ITO (see Fig. 1). Moreover, CNT has a much higher sheet resistance as compared with ITO. The probed sheet resistances of ITO on glass, ITO on PET and CNT on PET are 36  $\Omega$ /sq, 52  $\Omega$ /sq and 288  $\Omega$ /sq, respectively. As a consequence, solar cells based on CNT electrodes will need some different preparation process to develop these properties compared with the conventional ITO electrodes. An additional problem is that the CNT on PET is not stable when cleaning with usual organic solvent ultrasonic bathing. The acid etching isn't suitable for CNT film, either. To overcome these problems related with CNT electrodes, we choose O<sub>2</sub> plasma method for etching and use di-water for cleaning. It is also found that the HNO<sub>3</sub> treatment can decrease the sheet resistance of the CNT film. Furthermore, dissolving PEDOT:PSS in methanol can make the PEDOT:PSS layer coating on the CNT film easier.

Thus the preparation of solar cells with CNT electrode can be studied.

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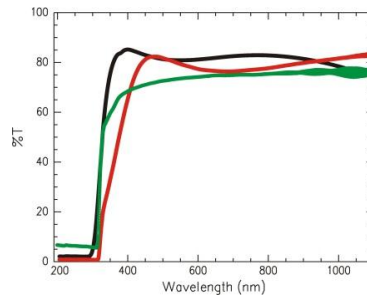


Fig. 1 Optical transmission spectra of ITO on glass (black), ITO on PET (red) and CNT on PET (green)



# Zinc oxide based hybrid films for applications in organic photovoltaics

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The drastic increase in daily energy requirements and environmental consciousness all around the world have motivated us to incline more towards green energy. In this context, solar energy serves as the most abundant source which has triggered the fabrication of photovoltaic devices in the past two decades for the generation of electric power. Organic solar cells as well as inorganic-organic hybrid solar cells have been developing which promise reduced fabrication costs, simple processing and employment of flexible substrates. Among them the hybrid solar cells are of greater interest as they provide the benefits associated with both the organic and the inorganic material.

Titania (TiO<sub>2</sub>) has been the most abundantly used inorganic material for the so-called dye sensitized (Grätzel) solar cells, providing efficiencies as high as 11 % [1]. However, extensive studies have revealed that zinc oxide (ZnO) with a direct band gap of 3.37 eV is a potential alternative for inorganic material in the solid state dye-sensitized solar cells because of its distinctive optoelectronic and photochemical properties [2]. It has also been shown that ZnO provides higher quantum efficiency and better activity in some cases as compared with titania. Additionally, ZnO absorbs over a larger fraction of the solar spectrum than titania. The results with ZnO based solar cells are quite promising and increasing with the combination of different hole conducting materials as indicated in figure 1 over the recent years [3].

Proper utilization of properties and applications of ZnO is highly dependent on ZnO morphology and structure. This has sparked the idea to design suitable nanostructured morphology of ZnO. A soft chemistry route based on sol-gel synthesis has been applied in the present study with the use of a structure directing diblock copolymer acting as a template. An example of the ZnO network structure obtained via such sol-gel route is displayed in figure 1. Moreover, several other nanostructured morphologies have been successfully obtained indicating the ease of tailor-made properties. For obtaining quantitative information about the film porosity and in-depth structure sizes, Grazing incidence small angle X-ray scattering (GISAXS) has been performed. A 2D GISAXS image of the corresponding ZnO morphology is shown in figure 1 as well. Ongoing investigations have been carried out to infiltrate the ZnO nanostructures with a suitable hole conducting material in order to proceed towards the final goal of fabricating solar cells with higher power conversion efficiency.

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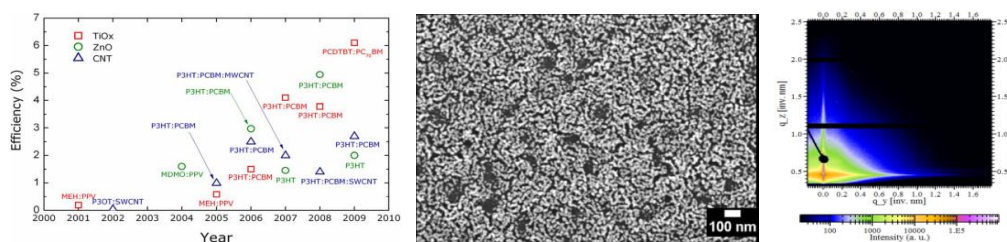


Fig. 1: (left to right) Development of the efficiency as a function of time as reported in [3], example of ZnO nano-morphology and related scattering pattern.

# Custom tailoring of titania thin films for application in organic photovoltaics

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The search for a solution to the world's energy provision is a challenge that gains more and more significance as we steadily use up our fossil fuels. Using the sun as an almost unlimited battery, photovoltaics became a promising candidate for a clean way to provide humanity with sufficient amounts of energy without harming the environment.

Today, the most common photovoltaic devices are silicon based. Despite being already commercially ready for use, silicon-based solar cells still are hindered by high production costs and complicated and energy consuming manufacturing processes. Next to those common p-n-junction solar cells another type has been found to be a technically and economically credible solar energy converter: the dye sensitized solar cells (DSSC). Its distinctive feature is a large-surface area titania film. Since the effective absorption cross-section of one dye molecule is too small, a large surface area is required to capture sufficient amounts of sunlight. By using a porous instead of a bulk titania film, the effective surface is increased by several orders of magnitude. This increase is directly transferred to the absorption of sunlight by the dye and hence to the performance of the DSSC. Along this route, by tailoring an optimized morphology the overall efficiency of the solar cell can be enhanced significantly. For the preparation of our films we use a block copolymer as a structure directing agent which is combined with a so-called good-poor solvent-pair-induced phase

separation coupled with sol-gel chemistry. By simple adjustments of the preparation conditions, various morphologies are accessible. Thus along this route, complex hierarchical structures can be custom tailored [1].

To add more functionality to the titania film superstructures are applied. The beneficial influence of superstructures has been successfully demonstrated in the past [2]. A light trapping effect can lead to enhanced absorption in the film which is a highly desirable property for photovoltaic devices. Using cost-efficient printing techniques the superstructure is applied to the titania film employing custom-designed masters.

In such systems, we perform thorough morphology investigations using various microscopy techniques like optical microscopy, scanning electron microscopy (SEM) or atomic force microscopy (AFM). Furthermore, reciprocal space analysis is performed with X-ray reflectivity (XRR) measurements and the advanced scattering technique grazing incidence X-ray scattering (GISAXS). Optical film properties are investigated with photoluminescence spectroscopy (PL) and UV/VIS and the film crystallinity is probed using X-ray diffraction (XRD).

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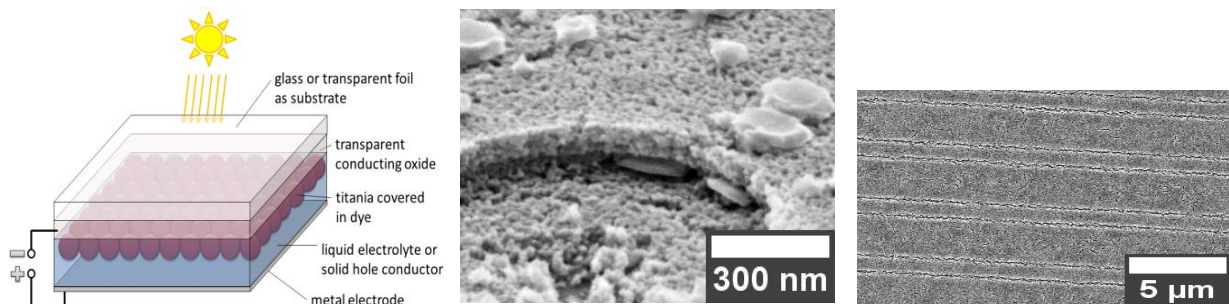


Fig. 1 (left to right): Sketch of titania based photovoltaic device, SEM close-up of layered titania foam, superstructured titania film with porous nanostructure

# Nanostructuring of titania thin films by combination of micro-fluidics and block copolymer based sol-gel templating for application in photovoltaics

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Inorganic-organic hybrid photovoltaics are one possible approach to tackle tomorrow's energy problems. These solar cells combine the advantages of the inorganic material like titania with the advantages of organic materials, which are cheap, easily manufactured and can be used on flexible substrates.

The principle setup of a hybrid solar cell is shown in figure 1 (left), where the light enters the cell through the glass substrate and a transparent conducting oxide (TCO) electrode. The charge separation takes place at the interface of titania and the organic hole conductor. Electrons are conducted in the crystalline titania towards the transparent electrode, holes are conducted in the organic hole conductor towards the gold top electrode. For effective charge-separation a large surface-to-volume ratio of the titania film is necessary. Sol-gel chemistry templated with a structure-directing micro-phase separation of an amphiphilic diblock copolymer solution results in a control of the structure on the nanoscale. Mostly the obtained structure is not very well ordered because of the fast reaction kinetics. Micro-fluidic cells, where small quantities of fluids can be controlled precisely, are widely used to control reaction kinetics.[1] Thus the combination of the two concepts, polymer templated sol-gel chemistry and micro-fluidics, is very promising to obtain titania structures with a higher degree of order.[2]

Real space investigations with scanning electron microscopy (SEM) reveal a pore structure with mesopores with a diameter of several tens of nanometers and macropores with a diameter of several hundreds of nanometers, as can be seen in the second figure for a structure derived from a sol-gel mixed in the micro-fluidic cell with a flow rate of 1 mL/min. Reciprocal space investigations with grazing incidence small angle X-ray scattering (GISAXS) have been performed to gain quantitative information on the structure in the volume of the film averaged over a large sample area. The scattering pattern of the titania structure derived from the sol-gel mixed in the micro-fluidic cell with 1 mL/min is shown in the third figure. From the scattering in  $q_z$ -direction information on the porosity can be obtained. For the samples prepared by a combination of micro-fluidics and polymer templated sol-gel synthesis the porosity is in the range of 75 to 80 %, which is a promising value for solar-cell applications. Together with an increased light scattering, as determined by UV/Vis spectroscopy, the obtained titania structures are highly interesting for applications in inorganic-organic hybrid photovoltaics.

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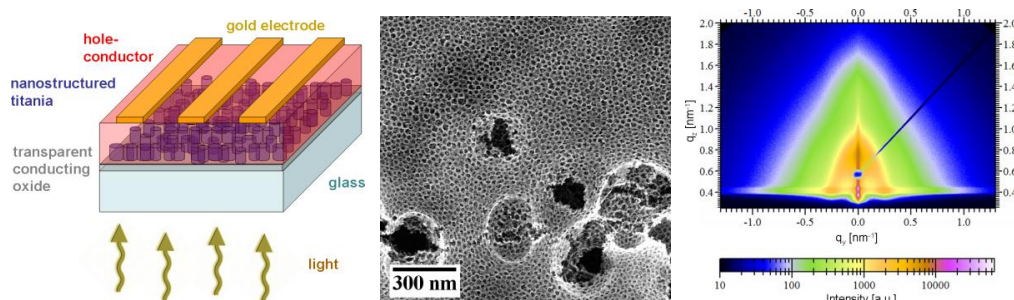


Fig. 1: (left) Sketch of solar device, (middle) titania nanostructure as probed with SEM, (right) example of 2d GISAXS scattering pattern probed at titania nanostructure.

# Simulation of Solar Powered Desalination Systems

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Humidification-Dehumidification (HDH) desalination plants are mostly used for the production of low quantities of water. This paper outlines the possibility of coupling HDH systems with solar concentrating solar power plants, enabling larger quantities of water to be produced.

Described herein is a numerical simulation model of a solar powered Humidification Dehumidification system. A numerical simulation tool (TRNSYS) was used in order to model the plant's components including different solar systems. The simulation model has been validated with measurement data from a prototype tested in Greece and Germany. Applying the simulation tool, now various configurations can be systematically investigated:

The first scenario focuses on the coupling of HDH systems with different solar collector types. Using the simulation model, the expected yearly water output for

different locations (e.g. Abu Dhabi, Dubai) can be calculated for different solar field sizes.

The cogeneration of water and electricity using solar power is of utmost importance for many regions in the world. The second scenario includes concentrated solar power plants (CSP) using parabolic trough collector fields, coupled with HDH systems.

Within the context of climate change and increasing demand for fresh water, solar powered systems gain more momentum, particularly when merged to create both electricity and fresh water.

Commercially available large-scale desalination technologies such as Multi Effect Distillation are used/proposed for most large-scale solar powered systems. Although HDH plants will not reach the Performance Ratio of large-scale systems, this desalination technology can be advantageous when coupling with large CSP plants.

# Crystallization and mesoscopic structures in polymer nanocomposites for batteries

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Energy storage is of key importance for the use of renewable energies. Polymer electrolytes mark a new class of materials for the use in energy storage systems such as batteries. Compared to the traditional Li-ion batteries with liquid electrolytes, they offer the advantage that the solid polymer does not leak. Moreover, smaller devices can be designed because thinner electrolyte layers become possible.

Poly(ethylene oxide) has been the polymer of choice due to its high conductivity when doped with Li salt [1,2]. At this, the crystallization of poly(ethylene oxide) must be hindered to achieve high conductivity. This has been achieved by adding ceramic nanoparticles which resulted in an increased conductivity [3,4]. In another study, Li doped PEO was combined with a (mechanically hard) polystyrene (PS) block for the use as polymer membranes in solid-state batteries and fuel cells [5]. Combining these two approaches, we aim at creating a mechanically rigid, nanostructured polymer electrolyte where the polymer matrix acts as a structure directing agent allowing for cylindrical or bicontinuous morphologies.

We focus on P(S-b-EO) diblock copolymers which exhibit the hexagonal cylindrical morphology with PEO forming cylinders in a PS matrix. We investigate the structures and thermal behavior of P(S-b-EO) which is doped with Li[N(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>] salt. We investigate the melting point and the degree of crystallinity of the PEO domains as a function of Li[N(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>] content using dynamic scanning calorimetry. The crystalline structures are characterized using temperature-resolved wide-angle X-ray scattering (WAXS). Small-angle X-ray scattering (SAXS) gives information on the hexagonal

structure, such as the distance and thickness of the cylinders as a function of Li[N(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>] content. Alternatively, breakout crystallization may result in the destruction of the cylinders and the formation of crystalline PEO lamellae.

Another important factor is the preparation route. In thin, supported films prepared by spin-coating, it has been found that only very minor contents of Li[N(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>] can be incorporated into the polymer matrix [6]. By investigating thick films and bulk material, we bridge the gap and identify the role of the substrate with respect to the miscibility of P(S-b-EO) and Li[N(CF<sub>3</sub>SO<sub>2</sub>)<sub>2</sub>].

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# Optimization studies for a more efficient converter unit for vanadium redox flow batteries

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Battery storage systems based on the vanadium redox flow battery (VRB) technology can contribute to integrate renewable energies into power grid. VRB offer free scalability and long cycle life. At the ZAE optimization studies for VRB with focus on the converter unit are conducted.

The converter unit is the main part and the cost driver of this kind of battery. Here, the liquid storage medium is pumped through for charge and discharge. The converter consists of electrochemical cells combined to a cell stack. Low cell resistance and good reactivity in terms of current density and reversibility are necessary for a good performance. The three crucial parts of the

cell are electrodes, bipolar plates and membrane. In current work different kinds of these components are implemented in a self developed, flexible test cell setup and evaluated.

A closer look at the electrodes reveals the possibility of increasing performance via activation of the carbon material of the electrodes – the mainly used material is graphite felt. This leads to the formation of surface groups that increase hydrophilicity and therefore wettability. Moreover, some catalytic effects for the vanadium redox reactions are ascribed to surface groups. In this poster activation studies of graphite felts are presented and discussed.



# Lithium-containing diblock copolymer thin films for solid-state batteries

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Rechargeable lithium ion batteries have been powering modern portable electronics for over a decade and a half, providing advantages such as higher energy densities, longer life-cycles and shorter recharge times compared to other rechargeable batteries. With the advent of the electric car due to steadily declining oil reserves, rising gas costs and efforts to reduce carbon dioxide emissions, research on lithium-based battery systems has intensified.

Typical lithium-ion batteries use a liquid or gel electrolyte with separators between the electrodes and the electrolyte. This has a number of drawbacks, such as the need for a solid encasing limiting the flexibility of possible applications and greatly increasing safety risks, and electrolyte damage and thus deteriorating performance over time. Solid-state polymer electrolytes address some of these issues by being robust, lightweight, non-combustible and shape-conforming, therefore allowing for flexible and light encasings, customized products such as very small batteries and improved safety aspects.

Semi-crystalline polyethylene oxide (PEO) has been the focus of research in this context as it solvates lithium ions, creating an ion-conductive membrane. However, PEO suffers from low mechanical stability due to the necessity of a good ion conductor to have non-rigid side chains, and quickly gives up even more stability at temperatures a bit higher than room temperature.

The solution to this problem has been to use systems consisting of self-assembling block copolymers, i.e. polymer chains consisting of two large blocks of distinctly different monomer units, such as PEO and polystyrene (PS).

These self-assemble to form a conductive PEO matrix containing non-conductive, rigid and glassy domains of PS, the latter ones providing the mechanical stability.

We study such PS-*b*-PEO systems in the form of thin polymer films as depicted in figure 1. The challenge of such devices being the optimization of the PS to PEO ratio to achieve optimal stability without sacrificing

conductivity, as well as optimizing the lithium salt content to the same end [1].

A major problem of PEO systems is the tendency of PEO chains to form crystalline domains which cannot conduct lithium ions, thus reducing overall conductivity. This tendency is believed to be favored by the presence of water in the films.

We attempt to address this problem by dispersing nanoscale ceramic particles in the films to form a nanocomposite membrane, as has been demonstrated before, e.g. [2]. Heating of this membrane above the glass transition temperature of PEO – roughly 60°C – followed by a cooling period should allow the PEO chains to re-arrange around the ceramic particles without crystallizing. Furthermore, we perform the manufacturing process in a glovebox, i.e. an inert nitrogen atmosphere with ultralow water and oxygen concentrations.

Structural characterizations of the nanocomposite films will be carried out using atomic force microscopy (AFM), scanning electron microscopy (SEM) and grazing-incidence small-angle x-ray scattering (GISAXS).

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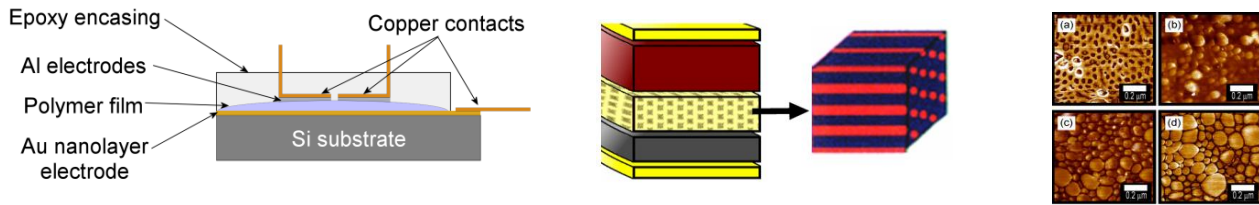


Fig. 1: (left to right) Sketch of a thin film polymer battery device, sketch of the used layered structure being the active part together with the diblock copolymer induced morphology of cylinders in a matrix and surface morphology of thin polymer film containing Li as probed with AFM.



# Challenges of battery systems in a tropical environment

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Energy storage for electric vehicles is still a common known problem. The key factors there are high prices – the battery pack with a Li-based technology causes almost 50% of the costs for an electric vehicle (cf. Fig. 1, [2] and [3]) –, high weight and a limited driving range. Using electric vehicles in a tropic environment like Singapore is even more challenging. Additional problems occur like high solar radiations, a high relative humidity of 70% to 80% and all-year average temperatures between 25°C and 31°C (cf. [1]). All these climate conditions cause additional, for Europeans often unknown issues in design and safety management of electric vehicles' batteries. At the TUM CREATE Centre for ElectroMobility in Singapore, a NRF1) sponsored joint interdisciplinary research project between TUM and NTU2), these challenges are faced and new safety mechanisms, adapted to the special climate, are developed and evaluated.

For battery management in a tropic environment one of the key issues is thermal management, as high temperatures deplete battery lifetime significantly. Furthermore, they are critically for the battery's conditions in the standing phase when active cooling systems are shut off. Therefore, passive cooling systems and a well chosen assembly are essentially. Additionally, different temperature monitoring techniques are applied: The first applied method is temperature sensing on the cell's surface. By placing a grid of temperature sensors on the cells a detailed temperature distribution model shall be created. Evaluating significant spots in the cell helps optimizing the amount of sensors to an applicable count.

For getting information of in-cell behaviors, temperature and pressure sensors are placed into the cells. Using both surface and in-cell data helps to create a 3-dimensional temperature model of the cell.

Algorithms for in-cell temperature estimation based on surface measurements can be derived.

Having an accurate temperature model of the cells gives the possibility of applying pre-conditioning methods for cells that can be used during charging. Additionally, within TUM CREATE a cell configuration on the material level for higher temperatures is determined. Present Li-based cell configurations are suitable for a temperature range between -20°C and +50°C (cf. [4]). Modulating the cell's suitable temperature range towards higher temperatures makes cells more applicable for tropic climate but at the same time less eligible for European climates. Having an accurate temperature model helps optimizing the cell's conditions for the chosen requirements.

Finally, cell-data are used for up-scaling towards battery modules and a whole battery pack. Surface temperature and in-cell measurement data are used to optimize the battery operation regime for temperature management while driving and standing, for charging methods, system monitoring, electrical management and safety management. The overall target is to maximize battery lifetime and to minimize safety risks.

#### Footnotes:

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- 2) Nanyang Technological University

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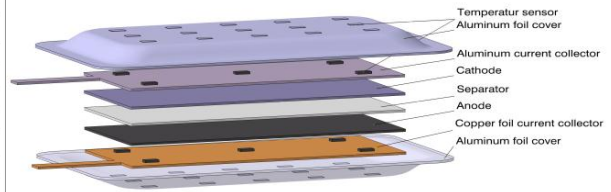
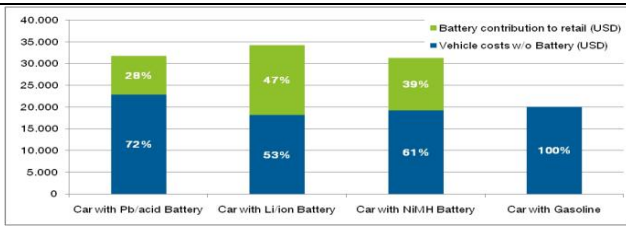


Fig. 1: Cost overview for the same car with different battery types/gasoline with a range of 200 km based on [3]

Fig. 2: Configuration of a pouch bag cell with in-cell and surface temperature measurement (Sebastian Bender, TUM CREATE)

# Li<sub>6</sub>PS<sub>5</sub>X (X = Cl, Br, I) as Solid Electrolytes in Lithium Ion Batteries

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The main challenge for electromobility is the development of high-performance lithium ion batteries (LiBs) with high durability. Particularly for post-LiBs like lithium-air and lithium-sulfur batteries, the development of lithium ion conducting solid electrolytes is critical, since they can prohibit the diffusion of contaminating species (e.g., CO<sub>2</sub> and H<sub>2</sub>O from the air in lithium-air batteries) from the cathode to the anode which would lead to rapid degradation of battery performance. Therefore, many types of solid electrolytes are being examined for their lithium-ion conductivity and their stability toward metallic lithium. One of the promising candidates for solid electrolytes are the halide lithium argyrodites, Li<sub>6</sub>PS<sub>5</sub>X (X = Cl, Br, I). According to

Deiseroth[1], these materials show a high lithium conductivity and are electrical insulators. Halide containing lithium argyrodites were synthesized and further properties were investigated at the chemistry department of TU München. Thermal behaviour is investigated by means of differential scanning calorimetry (DSC) and differential thermal analysis (DTA) and phase transitions are observed. Low and high temperature phases show different electrochemical behaviours. Impedance spectroscopy of the high temperature phase shows high lithium conductivity and the stability of these materials towards metallic lithium will be discussed.

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# The Product Selectivity of Oxygen Reduction Reaction on the Cathode of a Lithium-Oxygen Battery

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The demand for higher energy density storage devices for an efficient use of renewable resources has triggered the development of new Li-battery chemistry concepts. Due to the high theoretical energy density (3450 Wh/Kg) in comparison to the state-of-the-art Li-Ion (585 Wh/Kg)<sup>1</sup>, the non-aqueous Lithium-Air battery, although at an early stage of development, has the potential to become the ultimate electrochemical storage device, in particular in the field of electromobility. In water-free conditions, the oxygen reduction reaction (ORR) carried out in the presence of Li<sup>+</sup> ions during the discharge of a lithium-oxygen battery, could in principle lead to the formation of both Li<sub>2</sub>O ( $4\text{Li}^+ + 4\text{e}^- + \text{O}_2 \rightarrow 2\text{Li}_2\text{O}$ ) and Li<sub>2</sub>O<sub>2</sub> ( $2\text{Li}^+ + 2\text{e}^- + \text{O}_2 \rightarrow \text{Li}_2\text{O}_2$ )<sup>2</sup>. The product selectivity at the cathode of a lithium-oxygen battery should be influenced by the electrode material, including or not a catalyst, the discharge current density and the nature of the electrolyte. Oxygen consumption and XRD measurements carried out by several authors showed how Li<sub>2</sub>O<sub>2</sub> should be the main product on porous carbon cathodes<sup>2,3</sup>. In this study, the ratio between lithium oxide and lithium peroxide produced in the cathode of a lithium-oxygen battery during the discharge process is investigated by means of oxygen

consumption measurements. A system consisting of an electrochemical cell (Fig. 1) and a capacitance pressure transducer is filled with pure oxygen at ambient pressure and sealed (Fig. 2). During the discharge of the cell, the pressure of the gas phase is recorded (Fig. 3), and the pressure drop at the end of the discharge is used in order to calculate the amount of oxygen that was depleted. Therefore, the ratio between the quantities of the two products is calculated from the ratio between moles of electrons and oxygen involved in the battery discharge. Using this technique, the influence of different electrode materials, electrolytes and discharge current density is investigated.

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Figure 1



Figure 2

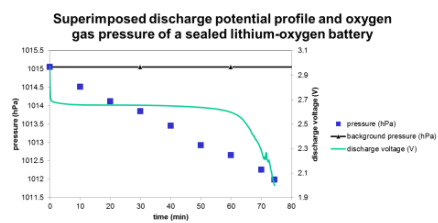


Figure 3

# Long-Lasting Energy Storage for Renewable Energies

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Because of the fluctuating offers of renewable energy, different storage possibilities are needed. As well as mid and long-time fluctuations especially short-time fluctuations have to be balanced by a storage system. To ensure high efficiency and continuous power supply of small isolated grids a special storage system is required. Grid-connected systems contain the possibility to compensate oscillation with other power plants. This possibility is getting more and more complicated because of the increasing part of renewable energies which makes a long-lasting storage system necessary. The aim of this interdisciplinary project is modeling and assembling a long-lasting cell embedded in an isolated renewable energy grid.

Guerfi et al. reported that a battery system consisting of Lithiumtitanate (LTO) and Lithiumironphosphate (LFP) is a promising candidate for a long-lasting storage system [1]. Figure 2 shows that it is very stable for more than 20 000 cycles. The insertion and deinsertion of Lithium-ions in both materials are highly reversible and occur with minimal volume variation of the crystalline cubic cell in contrast to graphite in the generally used Lithium-ion system. This characteristic is the determined fact for high stability and high cyclability. The cell potential is rather low, compared to conventional Lithium-ion batteries, making the LTO-LFP system with its low specific energy uninteresting for electromobility. For stationary applications the lower potential and the higher weight are negligible facts therefore the long lifetime and the high stability preponderance. Another

challenge of the system is its flatten of the potential curve shown in Figure 3 which makes it necessary to find a way to detect the state of charge of the cell.

The cells which will be assembled within the project consist of Lithiumtitanate coated on Copper anode and Lithium Iron Phosphate on Aluminum cathode in a Swagelok® T-cell. For electrochemical study a half cell of each electrode is mounted with Lithium foils as a counter and a reference electrode. The used electrolyte is 1 M Lithium Hexafluorophosphate (LiPF6) in a 1:1 mixture of Ethylencarbonate (EC) and Dimethylcarbonate (DMC). All cells are assembled under Argon in a glove box.

Generating a proper model of the storage system makes numerous test-runs necessary to identify and include the degradation parameters. To define the optimal size of the storage system and the optimal life-time parameters of the whole system, a higher prescinded model simulates the complete isolated renewable energy grid. Beneficial effects are estimated with combination of second life batteries and LTO-LFP systems. The benefit is seen in the different activation of the storage for short and long-time fluctuations.

This project is financed by the Nagelschneider Stiftung.

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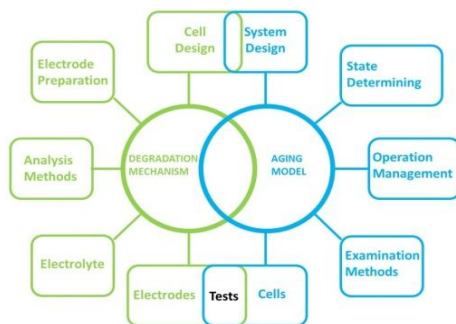


Figure 1: Overview of the interdisciplinary project

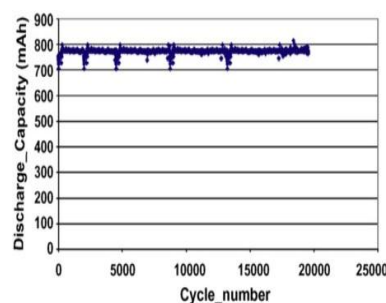


Figure 2: Discharge capacity of  $i_4Ti_5O_{12}/LiFePO_4$  system in an organic electrolyte with a discharge rate of 10C and a charge rate of 5C [1]

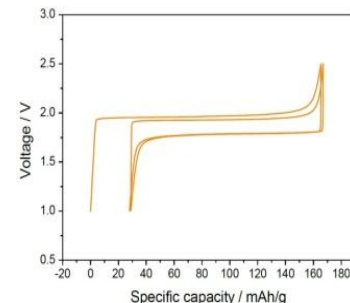


Figure 3: Potential curve of LFP against LTO [2]

# Associated Institute of Power Transmission Systems

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The power grids of the future will face a lot of new challenges including decentralization of power generation, strongly fluctuating power generation and new types of consumers e.g. electrical vehicles. The Associated Institute of Power Transmission Systems is researching on concepts and strategies on how to meet these challenges to secure a reliable and safe power supply.

Electric vehicles will drastically gain popularity and market share over the next few years due to the climate change and the scarcity of oil. The charging of the electric vehicles will increase the power demand and grid loading and therefore poses a new challenge to the power grid. On the other hand the batteries of the electric vehicles can help to even out the peak demand and congruence the energy generation and consumption. The Associated Institute of Power Transmission Systems is investigating concepts on integrating electrical vehicles into the power grid and analyzing the influence this will have on the power grid.

Due to governmental promotion, there is a fast growing amount of decentralized power units in Germany. With the assumption that small-scale photovoltaic power plants will use all available roof areas in the future, it is not possible to integrate the entire PV potential in

today's low-voltage distribution grids. In cases of increasing feed-in of fluctuating electrical power in low-voltage grids, transformers and cables can reach their loading limits. Moreover, the grid voltage can exceed permissible thresholds.

Local energy storages, which save the surplus generation, can be an alternative to grid reinforcement and can be essential for a stable and efficient energy network in the future. The Associated Institute of Power Transmissions Systems is investigating different scenarios for the optimal usage of energy storage systems in low-voltage grids with a high degree of decentralized generation.

Another option to avoid grid extension is the use of power electronic equipment. In this concept reactive power which is generated by solar power inverters is used to increase power capability and quality of the grid. Thus grid extension can be avoided in many cases or at least it can be delayed. Voltage fluctuations due to varying power input, e.g. caused by passing clouds, can be reduced. Additionally, inverters can be remotely controlled to compensate harmonic distortion and to improve phase voltage balance by feeding unsymmetrical currents into the three phases.

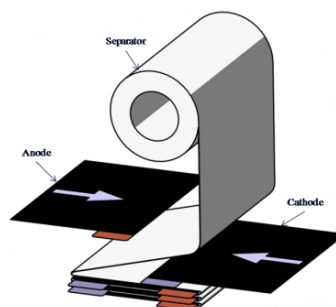
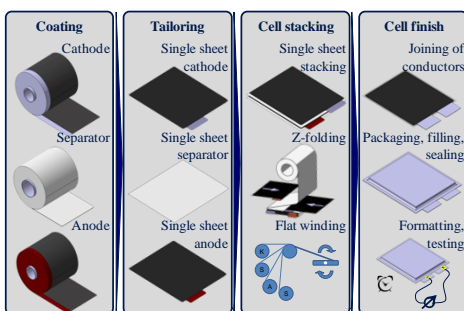
# Research and Demonstration Center for the Production of Large-Area Lithium-Ion Cells

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Electro mobility is a significant future trend justified by the efficiency as well as by the low emissions of electric drives compared to conventional internal combustion engines. One of the key issues to be solved in this context is the battery technology. In order to reduce battery costs advanced methods for the bulk production of lithium-ion cells need to be developed. Therefore, funded by the Federal Ministry of Education and Research (BMBF), the Institute of Machine Tools and Industrial Management (iwb) built up a demonstration center for the production of lithium-ion cells (DeLIZ). State of the art cell stacking technologies, such as flat winding, single sheet stacking and z-folding, have inherent drawbacks considering the final cell quality and the process yield. On the one hand, decollating and handling of nonrigid sheet type structures are complicate issues in the single sheet stacking process. On the other hand, the flat winding process affects the cell quality negatively by the applied process loads. Consequently, this paper evaluates different cell stacking methods taking into account

aspects of automation and process quality. Furthermore, an innovative z-folding process is presented as a result of these investigations. Due to the increased stacking speed and the optimized separator handling, the developed z-folding process is supposed to show a higher operating efficiency than conventional stacking processes. Besides that, the cell production is improved by laser based tailoring of the electrodes, providing a more flexible cutting process which is free of tool wear and which shows a reduced burr. Since each process step of the cell-assembly has a major impact on the quality of the finished lithium-ion cells, an overall quality management system is developed. After the identification of the important quality parameters, process latitudes can be defined. Furthermore, sensors for the measurement of these parameters can be selected and integrated into the demonstration center. The evaluation of the process data allows the optimization of the cell quality, the performance and safety as well as the energy efficiency and the process stability of the production system.



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# Green Navigation Systems for Electric Vehicles

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The depletion of fossil fuel reserves and the consequences of the climate change are major challenges of the new millennium. Electric vehicles (EVs) offer a potential contribution to the solution by their connection to renewable energy sources such as hydropower, wind power, bio fuels, solar energy and geothermal energy. Their batteries can be powered by these energy sources and they provide storage capacities to balance the power grid against the increased fluctuations in energy production from these sources compared to conventional sources like fossil fuels and nuclear power.

The drawback of EVs is their limited battery capacity, which currently only allows cruising ranges of around 100 to 200 kilometres. In addition, the charging of the battery pack of the EV can take up to several hours. The limited cruising range motivates two connected problems. First, an accurate prediction of the remaining cruising range becomes much more important than for fossil fuel powered cars with the currently limited number of charging stations and long recharge times. Moreover, to extend the driving range and to improve the probability to reach a charging station, energy optimal routes offer a possible alternative to shortest or fastest routes recommended by current navigation systems. Our Green Navigation system addresses these challenges by novel algorithms to determine the energy optimal route between two given locations and the

remaining cruising range. An example of a range prediction starting in Munich is shown in Figure 1.

The mean computation times of energy optimal routes and their energy savings compared to shortest routes for 100 randomly sampled source and destination vertices for classes with different air line distances are given in Table 1. The computation times to determine the cruising range for common battery pack sizes of EVs is below 1 second. The memory consumption in both cases can be neglected.

In contrast to common routing objectives like time and distance, energy is not only consumed while driving but energy can also be recuperated from braking, leading to a problem with a higher complexity in general. In addition, the required energy to drive a route depends on parameters of the road, vehicle, environment, behaviour of the driver and traffic flow. Finally, constraints posed by the battery render routes infeasible although its total energy costs might be below the battery charge. These challenges were met by modelling the energy optimal routing and range prediction problem within the shortest path framework [1]. An efficient solution was derived by modifying the A\* framework and utilizing domain knowledge, namely the law of conservation of energy to guide the search which reduces the problem complexity by one order of magnitude [2].



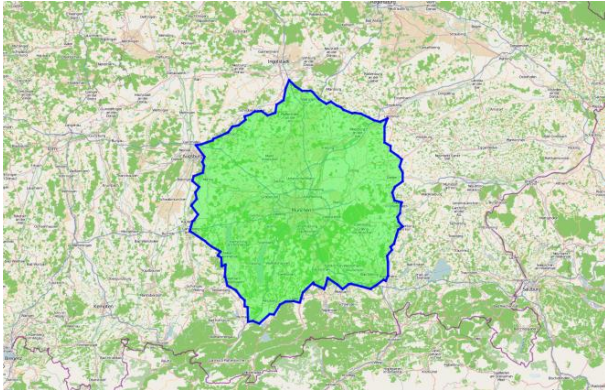


Figure 1. Cruising range prediction starting in Munich.

Air line distance [km]	Computation time [s]	Energy savings
]0, 50]	0.2	7%
]50, 100]	0.6	12%
]100, 150]	1.0	19%
]150, 200]	1.7	23%

Table 1. Performance of energy optimal route calculations.

This research is conducted within the eE-Tour Allgäu project dealing with the introduction of electromobility in a touristic region. The prototypic green navigation system GreenNav ([www.greennav.org](http://www.greennav.org)) is designated to be employed in the EV fleet in this project to offer tourists energy optimal routes and range prediction. In return, location data of the EV fleet augmented with energy consumption measurements are used to improve the energetic vehicle model. The estimated cumulative energy consumption with the energetic vehicle model with fitted parameters and the measured cumulative energy consumption of an EV on a test track are shown in Figure 2.

This system will also be employed in the electromobility project MUTE of the TUM as mobil device like the prototypic Android client shown in Figure 3.

Future research will incorporate more accurate traffic flow, driver behaviour and battery models to determine the energy consumption of an EV more precisely. Moreover, many parameters of these models, like the acceleration and deceleration behaviour of the driver,

can only be determined during driving and therefore adaptive models will be employed in the future.

In addition, we would like to expand our approach to the more general problems of car sharing and the shortest path problem augmented by the possibility to recharge on the route. Finally, stochastic models and multi-criteria optimization are planned to be part of our future work.

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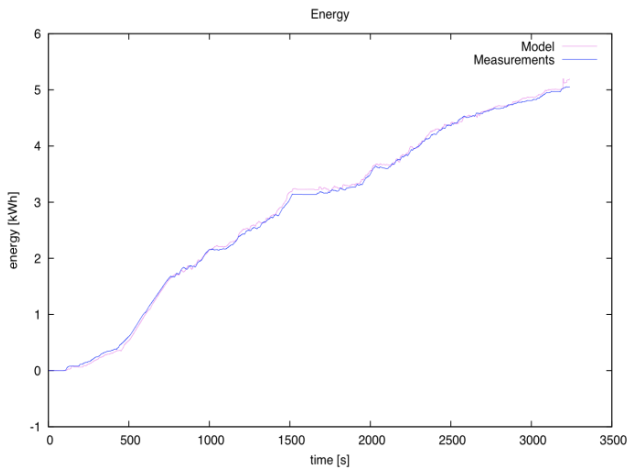


Figure 2. Energetic vehicle model with test track data



Figure 3. Android client of the GrenNav system.

## Smart Grids: Future Scenarios and related Business Models

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The increasing usage of renewable energy generation gives the great opportunity for a clean and sustainable energy supply for future generations. However, renewable energy generation will also exert remarkable strain on the energy system, especially on the electricity grid infrastructure. More than before the grid will have to be able to satisfy fluctuating energy demand and at the same time, they will have to cope with volatile energy supply from renewable sources. The modernization of the energy grid to a smarter bi-directional grid enables the components to communicate and balance the demand and generation more efficiently.

In this work the impacts of a smart grid on business models are analyzed in a methodological approach of trend research and future scenarios. In a first step the near future is analyzed, summarizing the status quo and identifying upcoming trends. An interdisciplinary approach ensures that technological, economic, social, political, legal and environmental trends are taken into account. In this analysis more than 80 trends have been identified. These trends give the basis for upcoming developments and future business opportunities.

In the second step the trends were clustered into specific categories and the main driving forces behind them are identified and evaluated regarding their impact and uncertainty in order to identify the relevant key drivers for different perspectives on the emerging smart grid industry (e.g. perspective of utilities, information and communication industries). Afterwards possible interactions and combinations of drivers are analyzed and combined to different scenarios that explain the industry structure and business environment of the future and thus serve as a framework to develop ideas for upcoming product and service ideas. Each scenario

describes a certain development for the upcoming 15 years and has a different anticipation of important framework conditions (e.g. customer needs, available technology and legislative regulations). The scenario analysis goes beyond the description of drivers and draws a concrete picture of the future.

Based on the scenarios, business models are developed and analyzed according to the approach of Osterwalder and Pigneur.

The poster shows the described methodological approach for the development of future scenarios regarding smart grids as well as one promising business model derived from a future scenario. The most important elements of a business model are described and a mockup illustrates how the product or service might look like in about 15 years.

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# Discrete dynamical systems as models for smart grids

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A major challenge in the operation of smart grids is fast and precise control. Sinks as well as sources in smart grids undergo rapid changes. The dynamics of many similar sinks are — up to a certain degree and at least on average — predictable and even manipulable. In contrast, a multitude of the sources are not: wind and sun follow the chaotic dynamics of weather.

There are very well developed and validated models for the processes within a power grid, based on ordinary and partial differential equations. In principle, the adaptation of control can be derived from these models. The drawback is the high computational burden that does not allow to determine an optimal control of large grids in real-time.

The aim of the present work is to come up with a discretization method for these large PDE/ODE models based on set oriented methods, and to describe

completely discrete (in time, space and state) dynamical systems that still incorporate the important features of the original dynamics. We allow for the loss of information and gain models that are much simpler than the usual ones and become accessible to very efficient and simple simulation techniques.

As a toy problem to develop and test these ideas, we consider the Fischer equation on the real line. The discretization scheme yields a structure resembling cellular automata, but the automata are non-deterministic in the sense of automata theory. We embed this structure in a classical cellular automaton with an augmented local state space. Methods similar to the construction of sub- and supersolutions yield the typical solutions we expect for the Fischer equation: especially, we find running fronts spreading over the grid with uniform velocity.

# Innotruck: The experimental vehicle of the IGSSE project “Diesel Reloaded”

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The Innotruck is an attempt of creating an extremely low CO<sub>2</sub> output goods transport vehicle, with the ability to integrate into and support the smart energy grids of the future.

The experimental vehicle platform was provided by the project leader Prof. Dr. Gernot Spiegelberg, a Rudolf Diesel Research fellow at the Institute for Advanced Study of the Technische Universität München.

A holistic approach to electromobility is being considered, with the focus being placed onto the system architecture, the energy management and the human machine interface. This approach encompasses a reduction in both development complexity as well as total cost of ownership.

The consumption of energy is optimized through the aerodynamic design and tires with an extra low rolling resistance. During the project the total energy flow within the truck will be analyzed and additional improvements will be implemented.

Energy management and distribution is deeply interwoven with selecting an optimal model for the operation of battery system and range extender.

35m<sup>2</sup> of photovoltaic panels developed by our partner BeBa Energie will power the comfort systems during the drive and provide clean energy while the vehicle is stationary.

The Innotruck is extremely streamlined, additionally boasting a completely flat vehicle base due to the

absence of pressured air containers. A constant air pressure is being stored in so-called plug-in axels, which serve as smart actuator units and have been developed

in the scope of a PhD thesis under the supervision of Prof. Spiegelberg.

The vehicle in itself represents a micro smart grid or an instance of the smart building concept. It is clear that the nature of energy generation and consumption will change drastically in the years to come, as demonstrated by the ever increasing number of electrical vehicles and clean energy sources. The energy grid has to become flexible and remain reliable, a feat made possible by mimicking the entire grid in entities such as Innotruck. Depending on the situation in the grid or on the consumer side, energy can flow in both directions enabling total personal mobility while not interrupting the overall network stability.

The recharge modules on both sides of the Innotruck are the key part of the fleet support capability, charging a maximum of 8 other electrical vehicles and increasing their operational range. The trailer will be equipped as a workshop, providing on-field maintenance in the events such as Zero Emission Race.

An installation of a retractable wind turbine on top of the vehicle is also planned, which can be activated when the vehicle is stationary.



# Modelling the Impact of Acoustic Pressure Waves on Auto-Ignition Flame Dynamics in Gas Turbine Combustors

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The transition from fossil and nuclear resources to renewable energies will ask for tremendous efforts and investments in the power generation sector in the upcoming years. Special attention has to be addressed to guarantee a sufficient electricity production at any time, what is a challenging task because of the high volatility mainly of wind-based power generation and the very limited storage capacity for electrical energy.

The use of combined-cycle gas power plants is considered as a strategic solution to facilitate the transition, as they allow very flexible operation (engine start-up < 20 min) at high fuel efficiency (up to 60 % electrical) and low specific CO<sub>2</sub> emissions compared to coal-based power plants. Furthermore, a promising new solution for high capacity electrical energy storage is based on synthetic methane production from surplus wind electricity.

As a consequence, the development of sustainable energy production also relies on the further development of a conventional technology such as gas turbines. This is one of the main motivations for the research initiative KW21 (“Kraftwerke des 21. Jahrhunderts”), with which the present research work is affiliated.

The major research activities in the gas turbine sector are driven by the needs for more efficient processes with lower pollutant emissions and extended fuel flexibility. This leads to an increase in compression ratio and the use of more reactive fuels, what significantly changes the operating conditions in the combustor, where auto-ignition processes start to play an important role.

From a methodical point of view, this evolution asks for a significant adaptation of existing analysis tools, such

as e.g. combustion models for CFD simulations, or flame dynamics models for the assessment of thermoacoustic stability. This work is related to the latter point, and presents an analytical description of a possible thermoacoustic feedback mechanism for auto-ignition flames, namely the impact of isentropic, acoustic pressure waves on auto-ignition chemistry and thus on the heat release rate.

In this context, fuel injected at a particular instant in time into the burner is assumed to contribute to the heat release at a later time. The interval between fuel injection and consumption, i.e. the ignition delay, depends in general on temperature, pressure and fuel concentration, and can thus be influenced by acoustics.

Hence, a quantitative description of heat release rate modulations caused by fluctuating ignition delays is presented. The delay time variations due to low amplitude isentropic pressure fluctuations are investigated using reactor calculations with detailed chemistry and represented by a sensitivity factor. Eventually an expression for the auto-ignition flame frequency response is obtained. Eigenmode computations with an acoustic network model show that variations of ignition delay caused by pressure fluctuations can result in thermoacoustic instabilities at elevated frequencies.

The present work is meant to give a representative example of the difficulties induced by new development trends and how these can be captured by advanced methodological tools in a multidisciplinary context involving chemistry, thermodynamics, and acoustics.

# Heat Pump in Electric Vehicles

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Because of the low storage density of today's batteries, the range of electrically driven vehicles is limited. The electrical drive unit as well as auxiliary equipment has to be powered from the battery. In relation to the range this should not be neglected. The largest auxiliary equipment in electric vehicles is the air-conditioning and heating unit. Because the heat loss of the electric machine is insufficient to heating-up the cabin, an electric heater is used. This may, in unfavorable conditions, expend up to 50 percent of the stored energy, so the range decreases accordingly. Up to 10 kW thermal power is necessary to heat the vehicle interior in the winter. In the case of cooling the cabin a thermal power up to 5 kW is to be provided by the air conditioning unit. In moderate climate zones, like Germany, the heating mode is the critical operation mode. In addition to the reduction of the heating and cooling demand, an efficient heating- and cooling technology is required to achieve an acceptable range for electric cars.

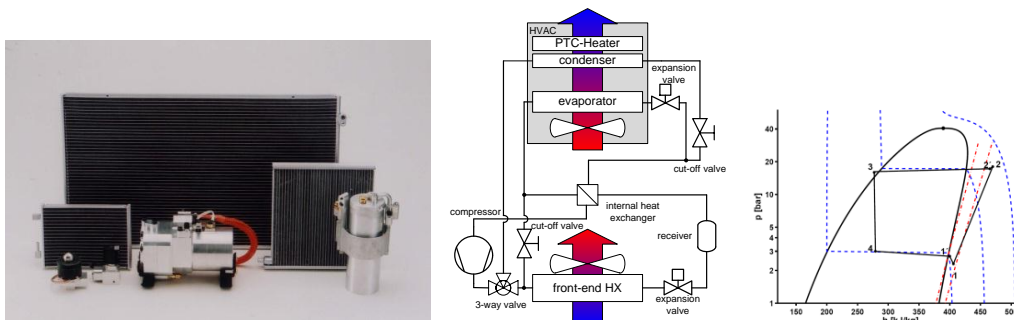
Using the air conditioning refrigeration cycle as a heat pump is one applicable and energy efficient possibility. An intelligent connection of the five main components: compressor, condenser, expansion valve, internal heat exchanger and evaporator enable a heat supply to the vehicles interior. Because of the localized heat exchanger additional valves are required to use the refrigerant cycle for cooling and heating. To avoid flash

fogging in the cabin a second heat exchanger operated as a condenser in the ventilation unit (HVAC) is necessary.

In most cases the environment is used as the heat source so that the heat exchanger on the car front is operated as an evaporator. In this operating mode a coefficient of performance (COP) of 2 to 5 is possible. At low ambient conditions an approximately 60° C warm supply air has to be created by the heat pump. That means the compressor has to overcome a very high pressure ratio. Its efficiency decreases rapidly and the COP of heat pump is nearly 1. This mode should be avoided.

A heat pump model is designed to compute the optimal operating points depending on the ambient conditions. Furthermore, three potential applicable refrigerants (R134a, R1234yf and R744) are compared to identify an ideal Air-to-Air heat pump for automotive application.

The results show the performance of the heat pump compared to an electrical heater and the energy saving in selected driving cycles.



# Reduction of heating loads for electric vehicle passenger cabins

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Due to the shortage of oil and strong carbon dioxide emissions of conventional vehicles, the electrification of the power train is a fundamental step towards sustainable traffic system. One challenging task in the development of electric vehicles is their thermal management. Components like the battery must be thermo-regulated very accurately. At the same time the conditioning of the passenger cabin requires high cooling and heating powers, which - when supplied by the battery - reduce the range of the vehicle dramatically. As the efficiency of the electric drive train is very high, in contrast to conventional vehicles, the waste heat is not sufficient for cabin heating. Therefore, new strategies are being explored to reduce the heating load and to fulfill thermal comfort with as little electric input as possible.

Depending on the climate conditions, heat and cooling loads of the passenger compartment can get relatively big. Conventional cars can handle heat loads up to 10 kW and cooling loads up to 5 kW. The heat load has, up to now, not influenced the energy consumption of vehicles, as this load could be covered by waste heat of the engine.

A thermal model of a passenger compartment is being computed the transient heat loads in dependence of the climatic and the operating conditions. Different bodywork layouts and options with improved insulation are compared in performance.

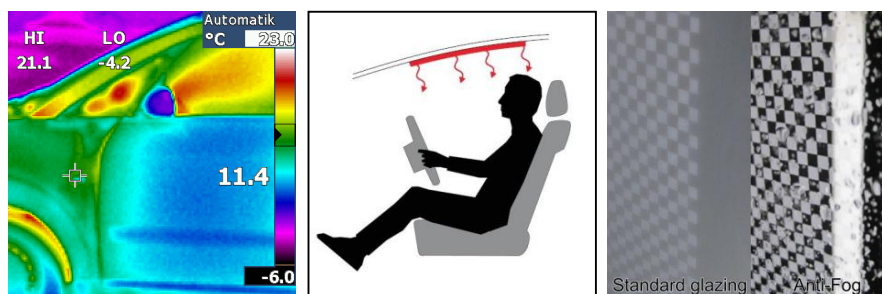
In cool climates most of the heat load arises from a relatively big ventilation mass flow of external air. The

ventilation number in vehicles can be an order of magnitude higher than in buildings. A high fresh air mass flow is necessary to avoid condensation of air humidity at cool window surfaces. Therefore, by preventing window fogging, the recirculation number can be increased and a significant part of the heating power can be saved. Strategies to avoid window fogging are being explored numerically and experimentally.

The second approach to reduce heating loads is to fulfill thermal comfort of the passengers with alternative heating methods. Instead of heating the complete air-volume of the cabin and heating the passenger by convective heat transport, heating is more effective, when transported to the human directly by radiation or thermal contact. In parallel to the calculation of thermal state of the bodywork, the thermal comfort of a passenger inside is determined. The influence of the bodywork physics (e.g. air velocity, surface and air temperatures) on human thermal physiology is represented, as well as the passenger's influence on cabin conservation equations.

The most promising measures to reduce heating loads are an improved insulation of the glazing, an enhanced recirculation ratio / reduced fresh air supply, and for the comfort approach radiant panel and seat heating, which allow a reduced air temperature at constant comfort.

Results of the calculation show that by a combination of several measures the necessary heating power can be reduced by more than 50 percent.



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# Towards an ecological perspective for energy efficiency in China's urban development

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In the last ten years, China has already developed itself as the largest energy consumer, the largest market for auto industry as well as the largest CO<sub>2</sub> emission country in the world. Its rapid urbanization and urban development pattern will to large extent influence the today's international efforts in energy supply and CO<sub>2</sub> emission reduction. At first, this paper tries to delineate the existing pattern of urban development in relation with energy efficiency. Based on the critical analysis, the strength, weakness and potentiality of this pattern will be discussed. Together with the discussion on current new symptoms in the national policy and in urban development practice, the author tries to raise a ecological perspective for energy efficiency. At last, a series of organizational and technical recommendations would be raised under this perspective.

The existing pattern in China's urban development has a strong hierarchical character with very limited goals set around the economic growth. Accompanied with the high speed of growth, this pattern is always criticized for its low resource utilization's efficiency and lack of coordination capacity for the synthesized effect in resource-friendly development because of its extremely centralized power structure. This situation has always

constrained the public participation and further social communication to develop the potentiality in energy efficiency and other related aspects for the sustainable development. As a result, the current efforts for energy efficiency e.g. building of Low Carbon City or reduction of CO<sub>2</sub> emission has reflected this structural flaw and should be improved both in organizational and technical aspects.

In the view of author, such existing pattern is seen as the obstacle for the popularization and utilization of today's technical progress for energy efficiency. A new ecological perspective for the urban development is raised as recommendation. In this meaning, the strength and potentialities of existing pattern e.g. in cultivating a relatively compact spatial structure will be utilized, so that the efficiency in energy supply and consumption could be achieved. At the same time, a series of decentralized adjustments will be discussed, so that the application of technologies e.g. Combined Heat and Power (CHP) and utilization of local regenerative energy resource could be integrated into the urban development process for sustainability.

# Simulation and Evaluation of an Energy Farm concept

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The share of renewable energies in the world's energy production is growing every year and so the demand for intelligent energy production / consumption systems is rising. As part of the "eE-Tour Allgäu" project the concept of an "Energy Farm" is discussed, simulated and evaluated. The power production of some important renewable energy sources – like wind and solar power – can be controlled only partially and relies much on conditions that can't be influenced while on the other hand a stable energy supply is crucial in today's society. A possible solution to that problem is the intelligent use of storage units for electrical energy – a field many researchers are working in today. Key to success is the combination of an intelligent power production, distribution and consumption to keep the stress on the electrical grid and the needed investments for the future energy supply as small as possible. As part of the "eE-Tour Allgäu" project the concept of an "Energy Farm" shall be developed and evaluated together with industry partners like John Deere and Allgäuer Überlandwerk (AÜW). An "Energy Farm" consists of one or multiple sources of renewable energies – e.g. photovoltaic or biomass – and one or multiple consumers of energy – like the household of the farmer and farm machinery/buildings. For storing electrical energy the lithium-ion batteries of hybrid drive train tractors shall be used as long as they are not needed for field work. Also additional energy storage

units are possible, if needed. The goal is to reduce the stress on the grid to a minimum compared to an uncontrolled system and use a maximum of the produced renewable electrical energy on the farm. So far the general design has been evaluated and discussed as well as a basic simulation of the farm has been set up. AÜW provided load profiles for different forms of renewable energy and John Deere contributed general usage profiles of tractors on a theoretical "model farm". This data combined delivers information about how much energy is needed every day e.g. for recharging the batteries of the tractors, and how much energy can be provided by the renewable energy sources. Together with different electrical storage sizes a power and energy need/surplus can be calculated for every day of the year. As next steps different combinations of energy sources and consumers shall be evaluated in combination with different tractor usage profiles to evaluate the economic efficiency and the actual benefit of such a concept. Together with an intelligent optimization control the stress on the grid shall be minimized and the self-consumption of produced energy shall be maximized. Another goal is to simulate the conglomerate of different farms of different sizes, to evaluate possible benefits. Also a market model shall be integrated in the simulation model to allow the optimization for economic efficiency.

# slowup@LANDSCAPES

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## slowup@LANDSCAPES - Renewable energy supply as a brick of designing sustainable landscapes Climate change and speed of life

Crucial for current global climate change is the difference in velocity between Nature and Culture, thus between speed of life on earth and speed of being live here and now.

So disregarding unforeseeable activities such as of volcanic or solar sources, natural changes proceed in a much slower way than cultural ones.

This impact of our “hurry up” mankind into any of these “slow down” natural processes has already been mirrored in the geological definition of the Anthropozän. (Paul Crutzen)

Within that definition, climate change is not the sole consequence. However, therewith many related coherences such as the role of renewable energy supply can be headlined together.

### This time - climate change is a matter of cultural stewardship.

Now, the main question remains:

How would we like to respond to this stewardship as a culture in our 21th century? Current discussed approaches like Geo-Engineering (NAS) focus very much on technical aspects. Thus again we discuss to influence in a way of “live”. But upon our cultural intend of sustainability: More justifying seem to be those approaches, targeting crucially the difference in velocity while being aware of the complexity of the biosphere as a system.

### slowup@LANDSCAPES as sustainable buffer

In this presentation we show, that a toolbox considering the three relevant factors already exists.

It is an adaptation of natural and cultural processes @ their velocity. At the same time it has been evolved through permanent cultural stewardship. Furthermore it is an active part of the system biosphere. Finally, if that toolbox has been designed for human demands and has so become environment, we start to call it: The Landscape.

Headlining climate change, slowup@LANDSCAPES provide “new landscape” classified by three types. As buffer they balance, hurry up or slow down nature- and mankind processes.

### “Timeout landscapes”

Our current forms of land use and settlement reply by short-term velocity of adaptation to consequences of climate change. The vulnerability towards the impact of climate change is immediately declining. The result of rising resilience wangles us the time, left to further adaptation of the velocities of Nature and Culture.

### “Decelerating landscapes”

Our environment acts as CO<sub>2</sub>-Circle and by mid-term velocity of mitigation our carbon footprint is reducing. Therefore current forms of land use and settlement are evolved and our energy is increasingly supplied by Renewables. Expanding this kind of CO<sub>2</sub>-Neutrality we extend our time slot reaching sustainability. Climate change is decelerated.

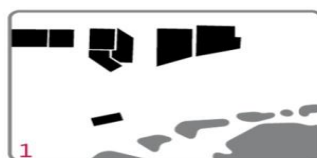
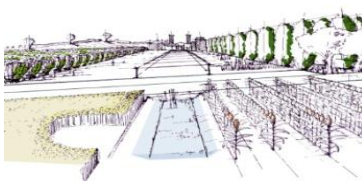
### “Decubancy landscapes”

By the long-term velocity of adsorption the environment operates as a carbon sink. This function is surely one among many other tools for climate gas treatment. The “decubation period”, until the CO<sub>2</sub>-concentration reduces actively assisted by these tools, ranges within the time span of cascade use till the assisted build-up of new fossil resources.

### “slowup” as a landscape design

Designed and evolved on the method of research by design we show our current research state of slowup landscapes in different regions of the world. Surplus and Synergy are two of our leading design principles for future landscapes and their environmental quality.

The design process is intended to be constantly influenced by related fields of research and focuses on general approaches how we, as landscapes architects, can face big scale landscapes with cultural stewardship towards climate change



1  
“Alpha Ventus” (im Bau) und Planungen



# Facilitating reforestation while producing food and energy crops – An agroforestry approach in Panama

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The accelerating deforestation caused by unsustainable land use has been recognized as one of the major causes for climate change, loss of biodiversity and long-term degradation of land. At the same time, growing world population and the rising demand for renewable energy lead to a higher land consumption. These opposing requirements call for an extensive scientific research on sustainable land-use systems that reduce deforestation, support the regeneration of ecosystems, provide income for the people and produce high-quality products for the national economy as well as the global market. Agroforestry systems, the combination of trees and agricultural products (crops or animals) might present an opportunity to meet these needs of future sustainable land uses. The research approach of the present study is to integrate understory crops in timber plantations to provide high-quality wood products (eg. Mahogany, Teak...) as well as food products (e.g. rice, maize, beans...) and renewable energy resources (e.g. soya) and allow more efficient use of land and labor in comparison to tree or crop

monocultures. In the course of the present project different understory crops were tested under six different valuable exotic and native tree species on three hectares in Eastern Panama. Initial tree growth and mortality has been evaluated in comparison to tree monocultures as well as optimal tree planting distances and light regimes.

The results indicate no significant differences in tree growth and mortality between agroforestry treatments and plots without association with arable crops, which leads to the conclusion that enrichment planting is possible without causing damage to the high quality timber trees. The enrichment of the six tree species with pigeon pea (*Cajanus Cajan*) even improved tree growth. The economic analyses of the different systems indicate their economic profitability and therefore complete the assessment of suitability of the agroforestry approach as a sustainable land use concept to improve traditional plantation forestry and offer alternatives for the production of energy crops.



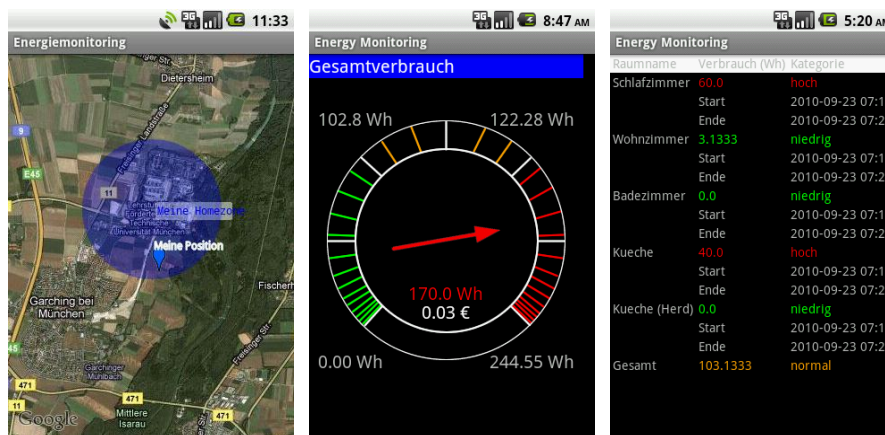
# Energiemonitoring und Steuerungsmethoden in privaten Haushalten mit mobilen Endgeräten

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Die Aufbereitung von Verbrauchsdaten wie Strom, Wasser und Gas / Öl ist für den Verbraucher ein wichtiger Faktor, um effektiv Energieeinsparungen betreiben zu können. Unterschiedliche Interessen sind dabei betroffen, beispielsweise die der Industrie, der Intermediären oder der Endkunden. Dieser Beitrag erfasst zunächst die technischen Möglichkeiten der Energieeinsparung und Aspekte von Gewohnheiten von Energienutzern, die in einer nach dem deskriptiven Design durchgeführten empirischen Studie ermittelt wurden. Im Weiteren zeigt die Arbeit mögliche Lösungsansätze für den nachhaltigen Verbrauch und Umgang mit Energie. Letzteres erfolgt über die Sensibilisierung des Kunden / Nutzers und eine damit verbundene Reduzierung des Verbrauchs. Dazu ist eine mobile Anwendung (Applikation) für das Android Betriebssystem prototypisch programmiert worden. Diese Applikation zeigt dem Nutzer verschiedene Darstellungsmöglichkeiten zur Identifizierung des Verbrauchs bzw. des Verbrauchers: Gesamtverbrauch in Form eines Tachos, tabellarische Übersicht des

Verbrauchs eines Stromkreises und eine „Homezone“. Befindet sich der Nutzer außerhalb der von ihm per GPS-Position festgelegten „Homezone“, so wird er an angelassene sicherheitsrelevante Geräte erinnert und kann diese (z.B. Herd) ausschalten. Ebenso ist ein Server entworfen worden, der die Daten für das Android System auswertet und aufbereitet. Insgesamt sind drei Teile (Messen der Daten, Auswerten / Aufbereiten der Daten, Anzeigen der Daten) des Energiemonitoringsystems in virtuellen Umgebungen implementiert worden. Abschließend wurde der Entwurf in Form einer Simulation systematisch evaluiert, um die Konzepte und Implementierung zu testen. Aktuell wird die Benutzbarkeit eines solchen Energiemonitoringsystems, für die in der Studie ermittelte Zielgruppe genauer untersucht. Ferner wurde noch ein Ausblick zur weiteren Entwicklung in diesem Bereich gegeben. Dieser Ausblick beschäftigt sich dabei im Kern mit der Sicherheit solcher mobilen Anwendungen.



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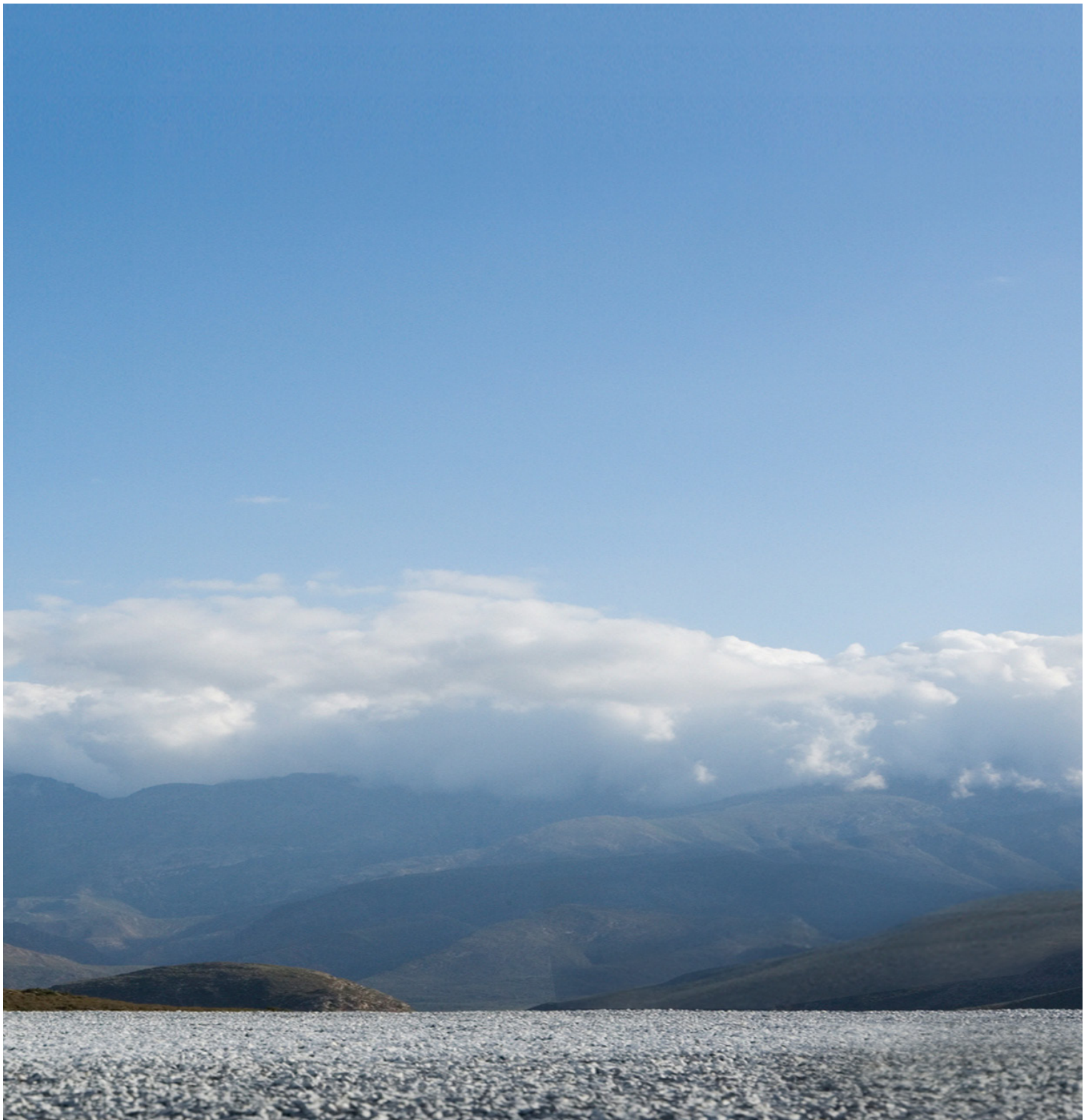
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**CPG** Center for Power Generation

 Science Center for Electromobility

**NRG** Network for Renewable Energy

**ENPB** Centre for Energy Efficient and Sustainable Design and Building