Munich School of Engineering

Technische Universität München

Energy Challenges – Germany 2050

2nd Colloquium of the Munich School of Engineering

28.06.2012

Contents

Oriented towards the „grand challenges“, the strategy of the Technische Universität München (TUM) is characterized by increasing its strengths with transdisciplinary research programs. One response of the TUM to the changing political landscape, most notably the decision of the German government to initiate the transformation of the energy system by 2050, was to join forces through the Munich School of Engineering (MSE). With its comprehensive cross-faculty research project TUM.Energy the MSE generates an amplified impact on research in the field of sustainable energy supply.

The first colloquium of the MSE, held in 2011, illustrated the wide thematic range of research activities at TUM in the field of sustainable energy supply. The focus of this second colloquium is to outline the transdisciplinary research potential at the TUM with regard to the innovations necessary for achieving the goals set by political decision makers. Natural scientists and engineers at the TUM will highlight their research output ranging from fundamental to application-oriented science.

I would like to invite you to join this MSE colloquium and participate in an exciting and interdisciplinary dialogue fostering new partnerships between researchers from the TUM and industry.

Thomas Hofmann
Vice President

Center for Power Generation

The Center for Power Generation (CPG) is an interdisciplinary working group consisting of institutes from TUM with research activities in the field of energy conversion for power generation. Besides efficient and innovative power plant technologies, the research spectrum 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.

Member institutes come from mechanical and electrical engineering as well as from the departments of chemistry and physics. Thus, a broad spectrum of expert knowledge is being brought together. One of the center's main purposes is its networking ability. Sharing information about research proposals, partner acquisition and active funding schemes is considered one of its fundamental goals by its members, thus enabling interdisciplinary cooperation.

To date 16 partners from 4 faculties share their expertise in the framework of CPG. New members are always welcome.

Network for Renewable Energy

The Network for Renewable Energy (NRG) is one of the four networks within the Munich School of Engineering (MSE). It acts as a platform for TUM researchers working on renewable energy projects independent of their discipline.

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 but also to foster an active communication between different research groups. The actively participating researchers are from various departments: Physics, Chemistry, Engineering, Electrical Engineering 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).

In this framework it was possible to form different larger scale project ideas over the last year. The most prominent project is currently TUM.solar, a key lab among 5 Bavarian key labs in the framework 'Solar Technologies go Hybrid' program of the Bavarian state Ministry. With a volume of approximately 5 million € scientists from the NRG are funded over 5 years to investigate hybrid systems of nano-materials for more efficient use of solar energy and photo-catalysis.

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

Science Center for Electromobility

The Science Center for Electromobility (Wissenschaftszentrum Elektromobilität – WZE) is a union of multiple 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 and fuel cell technologies to applied science developing innovative vehicle concepts. The successful completion of the MUTE project demonstrates the good relations between all partners in the Science Center for Electromobility. The subsequent project is called Visio.M and will reinforce the cooperation with the strong industrial partners participating in this project.

In TUM CREATE, a joint research programme with the Nanyang Technological University in Singapore, various partners of the Science Center for Electromobility go beyond the European borders and focus on research topics regarding electromobility in tropical megacities. Due to structural and climatic differences, an approach towards electromobility in this region must be completely different compared to the one in European countries.

As a member of the Munich School of Engineering (MSE) new interdisciplinary research cooperations are created regularly with the Science Center for Electromobility. Due to the flexibility of electric vehicles regarding their source of energy, there are multiple opportunities to use synergies between electric vehicles and other power sources or consumers. In order to explore and use these synergies, the Science Center for Electromobility is an important pillar of TUM's energy research for 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 motivated by the demand for the de-compartmentalization of the conventional engineering disciplines: the combination of interdisciplinary research and cross-faculty teaching. The teaching department of the Munich School of Engineering (MSE) provides currently three degree courses with the emphasis on an interdisciplinary education in the field of engineering sciences and is institutionalized as an Integrative Research Center with doctorate-granting rights. Talents in mathematics, natural science, and medicine get the chance to have a deep look on both, results of fundamental research in engineering and science as well as entrepreneurial viability of new technologies. This combination opens the MSE-graduates great professional opportunities in the interdisciplinary business fields of the future.

Since the winter semester of 2010/11, the MSE provides the bachelor course Engineering Science and the master course Industrial Biotechnology; in autumn 2012 the MSE starts the second master course Human Factors Engineering.

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.

By the course Human Factors Engineering (Master of Science) students get experts in terms of conception, implementation, and benchmarking human machine interaction concepts in the fields of automotive, aerospace, sports equipments, production, and software configuration. At the end of this study program the graduates are able to establish different kind of interaction principles and interaction technologies, to design specific grades of automation as well as to plan, to realize, and to evaluate the associated validation experiments.

Programme

8.00 - 9.00 am
Registration

9.00 - 9.15 am
Opening
Thomas Hofmann, VP Research & Entrepreneurship TUM

9.15 - 9.45 am
Keynote Speaker
Paul van Son, CEO Dii GmbH

9.45 - 11.00 am
Session Chair: Hartmut Spliethoff, CPG MSE

Future Power Plant Requirements
Christian Schuhbauer, Institute for Energy Systems

A Long-term Power Market Model
Matthias Silbernagl, Chair of Applied Geometry and Discrete Mathematics

Solid Fuel Gasification an Old Technology with Modern Challenges
Federico Botteghi, Institute for Energy Systems

11.00 - 11.45 am
Poster Presentation/Coffee Break

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

"In-operando" Neutron Scattering Studies on Commercial Li-ion Batteries
Anatoliy Senyshyn, Neutron Research Source Heinz Maier-Leibnitz (FRM-II)

Direct Carbon Fuel Cell
Michael Werhahn, Institute of Interfaces and Energy Conversion

Advances in Nanostructuring of Titania Thin Films for Dye-sensitized and Hybrid Photovoltaics
Monika Rawolle, Chair of Functional Materials

1.00 - 2.30 pm
Posterpresentation/Lunchbreak

2.30 - 3.45 pm
Session Chair: Werner Lang, ENPB MSE

Harvesting Solar Energy: DFT Studies of Organic Photovoltaics and Photo-catalytic Water Splitting
Harald Oberhofer, Institute of Theoretical Chemistry

Game Theory Approach for Interactive Wind Farm Control
Arman Kiani, Institute of Automatic Control Engineering

Smart Wind Turbine Rotor Blades
Liuz da Rocha-Schmidt, Institute of Lightweight Structures

3.45 - 4.30 pm
Poster Presentation/Coffee Break

4.30 - 5.45 pm
Session Chair: Markus Lienkamp, WZE MSE

Early Building Design: Heating and Cooling Plant Approach the Architect
Milica Grahovac, Institute of Energy Economics and Application Technology

System Modeling for Energy-efficient and Sustainable Building Design and City Planning
Philipp Geyer, Institute of Energy Efficient and Sustainable Design and Building

Smart Grid Demonstrator of a Future Office Prosumer
Denis Bytschkow, fortiss – Affiliated Institute to TUM

5.45 - 6.00 pm
Summary of the Day

6.00 - 6.45 pm
Keynote Speaker
Daniel Hofmann, Energy Sector Siemens AG

6.45 - 9.00 pm
Poster and Presentation Award/Colloquium Dinner

2 Oral Presentations

Future Power Plant Requirements

Christian Schuhbauer[a], Hartmut Spliethoff[b]

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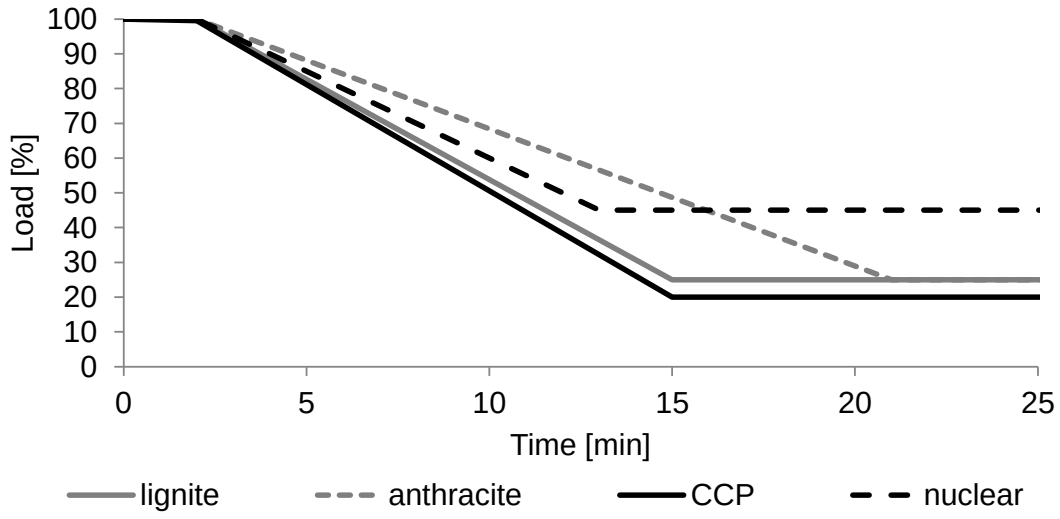
One of the main challenges of the 21th century is to ensure an economical, ecological and confident energy supply. The last years have shown, that these parameters are different evaluated and they are also weighted more dynamic. The Federal Government has finalized a bill for the national energy concept on the 28th of September. The concept which includes nine points covers renewable energies, energy efficiency, infrastructure of the electrical network as well as energy supply in the European Union and questions to the acceptance and transparency. Guidelines reach to 2050 to open the doors for renewable energies to achieve the aim of a reduction at 80 % of the greenhouse gas emissions in the industrial states. The coming abandoning nuclear phaseout whips up the public discussions of the future power supply. The questions are:

- How far are renewable energies able to replace nuclear power?
- How long does it take?
- How many fossil energy carriers are used?

With the discussed aims to extend renewable energies in energy supply it becomes clear, that in the medium term (2020 to 2030) the nuclear power has to be substituted in large part with conventional power of coal and gas in Germany or with import of electrical current of the European neighbors.

The contracts‘ frame should define the impact of the renewable energy expand on the electrical current production in Germany and the demands of conventional power plants as well as the future power plants and their qualification to load balance. The discussion is based on the aims of the energy concept of 2010. The expand aims for renewable energies won’t differ much in the medium term (2020 to 2030). The long-dated aims to 2050 also won’t differ much because of the nuclear phaseout.



A long-term power market model

Dipl.-Math. Matthias Silbernagl

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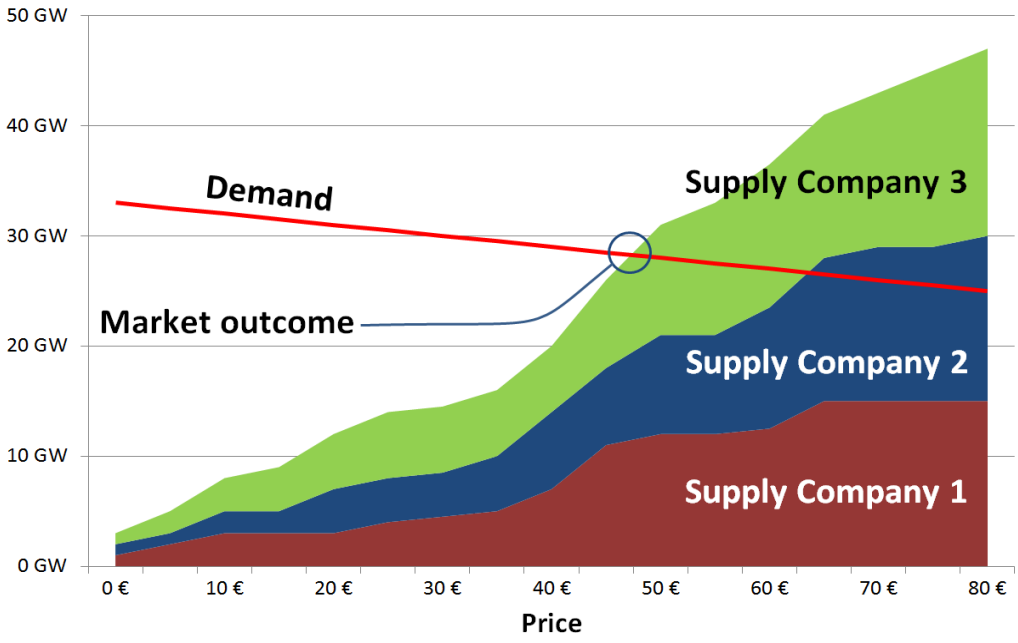
The deregulation of the energy market in the last two decades has attracted the researchers' attention, as electricity producers constantly needed to optimize their production to stay competitive. The raising volatility in energy production, mostly due to the increased use of renewable resources, even increases the potential for optimization and therefore the importance of power market models.

The target of our power market model is to provide long-term forecasts for the electricity price and for the usage of different production technologies. These forecasts are essential for power generating companies (*GenCos*) when devising long-term strategies.

The promotion of energy production from renewable resources has changed the market situation significantly, and will continue to do so in the future, making statistical models unsuitable for long-term analysis. As common in the literature, we therefore use the game theoretical concept of Nash equilibria to predict the behavior of the market; i.e. model outcomes are characterized as stable market situations, in which no GenCo has an incentive to change their strategy.

Models of this type have been very restricted in the level of detail in modeling the power generating units or in the implementation of the GenCos' strategies – in particular, the GenCo's strategy is usually modeled by only two variables, and the operational state of the generating units (off/starting/on) is usually not considered.

We model the strategy of the GenCos as a piecewise affine linear supply function, which describes how much each GenCo is willing to produce at a given price. The profit maximization problem of a single company is modeled as a Unit Commitment problem using Mixed Integer Programming. The model includes binary on-off variables for each generating unit, multiple periods, downtime-dependent start-up costs and the volatility of renewable energy production.



Solid fuel gasification: an old technology with modern challenges: Investigation and Research at the Lehrstuhl für Energiesysteme (LES)

F. Botteghi[a], C. Erbel, C. Kunze, M. Losurdo, M. Nakonz, R. Rück, H. Spliethoff

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For solid fuel gasification is intended that chemical process which converts the primary energy carrier (biomass, coal and derivatives, petroleum coke) in a synthesis gas mainly formed of H_2 and CO which has a big variety of applications. In the case of power production, the big advantage of this process is that, respect to the conventional firing where the pollutant are usually removed during and after the combustion, the syngas can be cleaned and purified before it is used, resulting, in the case of mere combustion, in a theoretically pollutant free process. The gasification of solid fuel, especially wood, coal and coke was developed during the 19th century when the energy demand, due to the industrialization, was dramatically increasing. The first application of this technology was to produce the so called “water gas” for street illumination. This gas was obtained blowing steam on glowing coal resulting in a gas rich in H_2 and CO_2. During the Second World War, applications for substituting conventional fuel in the automotive sector were developed; integrated coal gasifier were mounted on trucks to provide fuel. One of the most important Challenge for this technology today is to provide a reliable, cost effective, power generation system, the so called IGCC power plant (Integrated gasification combined cycle). This design takes advantage of the high efficiency achievable with a conventional combined cycle fired with natural gas, coupling it with a solid fuel gasifier enabling lower level of pollutant emission and the application of CCS technologies to avoid the CO_2 being released directly in the atmosphere. The research activities carried out at the Lehrstuhl für Energiesysteme on this thematic are widespread. In this Paper we present the investigations as well as the methodologies and the experimental rigs and instrumentation. The research efforts are focused, on the experimental basic understanding of the phenomena and the influence of thermodynamic parameters such as temperature and pressure by the mean of a pressurized entrained flow reactor capable of pressure up to 50 bars and temperature up to 1800°C. Other experimental rigs are present at the department such as pressurized thermobalances, a wire mesh reactor and a drop tube furnace. Computer simulations also play an important role in our research: on the one hand CFD simulations are run to better understand the influence of various parameters (geometry, velocity field, temperature and pressure) on the process supporting experimental activities, on the other hand overall cycle simulations are carried out in order to study the feasibility of new plant configurations taking into consideration also the economics involved. Our Research is framed within the project Hotvegas, financed by the German ministry for Economic (BMWi) and industrial partners i.e. Siemens, Rwe, EnBW, Air Liquide and Vattenfall.

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"In-operando" neutron scattering studies on commercial Li-ion batteries

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Due to the rapid progress in the field of portable electronic and electric vehicles there is an increasing demand for smaller size, larger capacity, lighter weight and lower priced rechargeable batteries. Nowadays the Li-ion batteries are considered as the predominant battery technology due to their high voltage, high energy, good cycle life and excellent storage characteristics. However, despite their overall advantages, Li-ion cells have some drawbacks, which can not be overcome and require systematic and detailed research, e.g. on issues concerning safety, cost, stability of electrode materials, capacity optimization and cell integration. Among various approaches towards a further improvement of battery technology, the characterization of the entire battery system during electrochemical cycling seems to be the most promising one as it gives unique information about processes occurring inside the battery "live". By definition, such type of "in operando" experiment performed on real industrial cells should be non-destructive keeping all battery constituents under real operation conditions. In those ways any risks of materials oxidation, electrolyte evaporation or battery charge changes are eliminated. In this sense neutron scattering due to its unique features is an outstanding tool often having no alternative, when characterization of complex Li-containing systems is under discussion [1]. The high penetration depths of thermal neutrons suits perfectly for non-destructive studies; the capability to localize light elements/isotopes (e.g. hydrogen, lithium) provides excellent phase contrast; the neutron scattering lengths not dependent on $\sin(\theta)/\lambda$ give accurate structure factors leading to precise bond-length and Debye-Waller factor analysis along with exact determination of lithium diffusion pathways.

A combination of available neutron scattering techniques permits the monitoring of evolution on various battery parts on different scale levels. The details of battery evolution on nanoscale have been obtained using high-resolution monochromatic neutron powder diffraction (instrument SPODI [2]), whilst features of the battery organization and details of its evolution on micrometer scale have been visualized using neutron radiography and tomography (ANTARES facility [3]).

The current contribution primarily concerns effects of fatigue processes in lithium ion batteries (which are of general importance for the battery development purpose) on the evolution and performance of Li-ion batteries. Results of combined electrochemical/neutron scattering studies performed on a batch of commercial 18650-type cells based on $LiCoO_2$ cathode and exposed to extensive cycling under controlled temperatures (25°C and 50°C), revealed their prominent fatigue. Effects of fatigue on the crystal structure, phase composition, bond length and microstructure of both cathode and anode electrode materials has been evaluated by the full profile Rietveld method.

The Li-intercalation into different electrode materials (graphite and $LiCoO_2$ for the current case), its details and kinetics, phase coexistence and material performance, is yet another important aspect of Li-ion battery technology. The application of high resolution neutron powder diffraction in a combination with neutron imaging and electrochemistry for studies of the battery evolution during slow charge/discharge unravel novel details of Li intercalation in the commercial Li-ion batteries, which will be presented in brief.

References:

[1] A. Senyshyn, M.J. Mühlbauer, K. Nikolowski, T. Pirling, H. Ehrenberg, "In-operando" neutron scattering studies on Li-ion batteries, J. Power Sources 203 (2012) 126-129

[2] M. Hoelzel, A. Senyshyn, N. Juenke, H. Boysen, W. Schmahl, H. Fuess, High-resolution neutron powder diffractometer SPODI at research reactor FRM II, Nucl. Instr. Meth. A 667 (2012) 32-37

[3] http://einrichtungen.physik.tu-muenchen.de/ antares/

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Direct Carbon Fuel Cell for Sustainable Electricity Production

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Conventional electricity production based on carbon containing fuels like coal involves a number of energy conversion steps. Direct conversion of chemical energy of the fuel into electricity can be achieved in a direct carbon fuel cell or battery. Electrochemical conversion of carbon is attractive because of the high theoretical conversion efficiency around unity, which is almost temperature independent as shown in figure 1. Carbon as fuel has a high energy density, is easy to store and readily available.

Several DCFC (direct carbon fuel cell) concepts employing molten carbonates, molten hydroxides or solid oxides as electrolytes have been reviewed by Cao et al. in 2007 [1]. These concepts use pure carbon or even coal. One drawback associated with molten salts is corrosion at elevated temperatures. This can be avoided by using a setup, where a porous carbon structure is in direct contact with the anode side of a solid oxide fuel cell [2]. Here, carbon black/ soot with electrical conductivity serves as fuel and part of the anode.

For this configuration, conventional anode design is not optimal. As solid carbon reacts only at the anode surface and not within the porous 3D reaction zone like fluids, a porous current collector layer is not applicable and porosity of the anode only reduces the ionic and electronic conductivities. Therefore a dense anode layer and a new current collector concept need to be developed. To increase the voltage efficiency with enhanced kinetics suitable catalyst materials have to be identified and integrated into the anode.

A first simple approach is a dense CGO (ceria doped with gadolinium oxide) layer as anode. At temperatures higher than 700°C, CGO becomes a mixed (ionic and electronic) conductor. Figure 2 displays a SEM (scanning electron microscopy) picture of the cross section of a CGO layer on top of a YSZ (zirconia doped with yttrium oxide) electrolyte. Ceria has proven catalytic activity in SOFC anodes and in catalytic soot oxidation from diesel exhaust gases [3]. At the anode, several reactions can occur as shown in figure 3. In this work, characteristic current-voltage curves are recorded in He, CO and CO_2 purge gas atmospheres at temperatures from 750 to 950°C.

1. D. Cao, Y. Sun and G. Wang, J. of Power Sources, 2007, 167, 250-257
2. S. Nürnberger, R. Bußar, P. Desclaux, B. Franke, M. Rzepka and U. Stimming. Energy Environ. Sci., 2010, 3, 150-153
3. S.P.S. Badwal and F.T. Ciacchi, Ionics, 2000, 6, 1-21

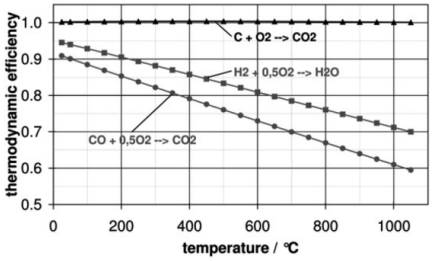

Figure 1: Thermodynamic efficiency for electrochemical oxidations [2]

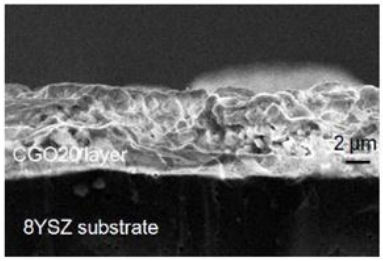

Figure 2: SEM cross section of CGO anode layer on YSZ

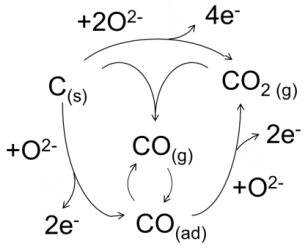

Fig. 3. Possible anode reactions

Advances in nanostructuring of titania thin films for dye-sensitized and hybrid photovoltaics

Monika Rawolle[a], Martin A. Niedermeier, Kuhu Sarkar, Philipp Lellig, Jochen S. Gutmann, Thomas Fröschl, Nicola Hüsing, Jan Perlich, Stephan V. Roth, Peter Müller-Buschbaum[b]

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In the course of an ever increasing demand of energy and the call for renewable energies, the usage of the solar energy available on earth as in photovoltaics is one possible way to meet the challenges. At the moment, the share of photovoltaics on all the available renewable energy sources is still very low, indicating that there is still a huge growth potential.

The most common technologies in photovoltaics are silicon based. These technologies have disadvantages, like high material costs, high temperature steps in production, and therefore a long energy pay-off time. A lot of material is needed for the rather thick silicon films. In addition, the resulting silicon cells are mechanically inflexible, thereby limiting possible application areas. Furthermore, the efficiency drops drastically with increasing solar cell temperature.

These challenges can be tackled by organic photovoltaics, as conducting polymers have the potential to be comparably cheap and easy to manufacture. Moreover, the organic materials can be used on flexible substrates. Flexible solar cells, for example on plastic foils, allow for very cheap production of the solar cells for example by roll-to-roll printing. Furthermore, as the cells have to be rather thin, not much material is needed. Even the issue of temperature dependency is improved, as organic solar cells perform better at elevated temperature, exhibiting higher efficiencies.

In addition to purely organic photovoltaics, the combination of the organic materials with a cheap inorganic semiconductor like titania or zinc oxide promises the same improvements. The resulting solar cells are called hybrid solar cells or, if an additional layer consisting of a dye as sensitizer is applied, dye-sensitized solar cells.

In the very thin film solar cells, nanostructures of the active materials are necessary. We have developed several novel pathways to create the nanostructures in the film and also to control the setup of the complete solar cell device.[1],[2] Figure 1 shows examples of titania based dye-sensitzed solar cells, both on glass and on a flexible plastic foil.

In our contribution we want to present the advances in the field of hybrid and dye-sensitized solar cells. In particular, possible nanostructure creation routes will be detailed.

[1] M. Rawolle, M.A. Niedermeier, G. Kaune, J. Perlich, P. Lellig, M. Memesa, Y.-J. Cheng, J.S. Gutmann, P. Müller-Buschbaum, *Chem. Soc. Rev.* (2012), DOI: 10.1039/c2cs15321a.

[2] M. Rawolle, M.A. Ruderer, S.M. Prams, Q. Zhong, D. Magerl, J. Perlich, S.V. Roth, P. Lellig, J.S. Gutmann, P. Müller-Buschbaum, *Small* 7 (2011), 884.

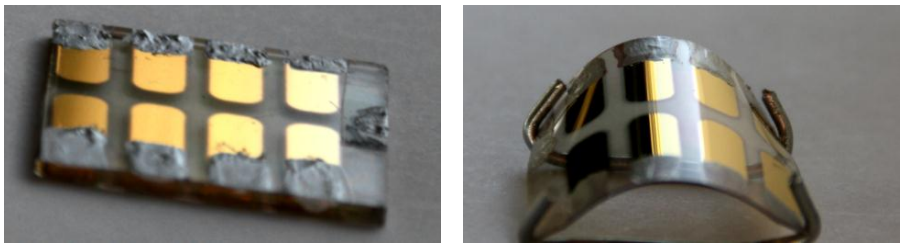

Fig. 1: Examples of a dye-sensitized solar cell on a glass substrate (left) and on a flexible substrate (right).

Harvesting solar energy: DFT studies of organic photovoltaics and photo-catalytic water splitting

H. Oberhofer[a], J. Blumberger[b], K. Reuter[c]

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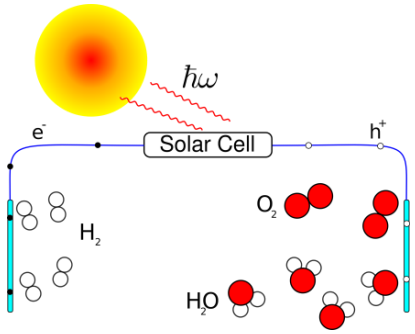
The sun is the largest provider of renewable energy in the solar system. Yet, so far directly harvesting solar energy constitutes only a small part of the world's energy supply even compared to other renewable energy sources. In our contribution we will discuss our theoretical research on two promising methods which could change this.

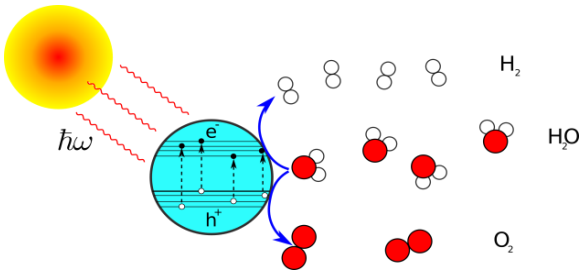
Organic solar cells

Organic solar cells are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. One of the loss mechanisms is inefficient charge transfer in the semiconducting layers. To gain atomistic insight into this process, we used advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified fullerene crystals, which form in the nano-crystalline domains of the n-type semiconducting layer in organic solar cells. Based on the DFT results we employed a kinetic Monte Carlo (kMC) model which allowed us to predict macroscopic electron mobilities, which are also accessible to experiments.

Photo-catalytic water splitting

We will also discuss our ongoing efforts in the field of photo-catalytic hydrogen production. Molecular hydrogen is a promising alternative to batteries when it comes to energy storage in that it can, in highly compressed liquid form, provide much higher energy densities than all current battery designs. We will report on our DFT based research on photo-catalytic water splitting on titanium dioxide semiconductors, nano-patterned with small (3-20 atom) gold nano-clusters. We investigate the suitability of these clusters as co-catalysts for the water oxidation reaction and identify trends with respect to cluster size. The aim of these efforts is to understand the mechanisms involved and their dependence on system structure, enabling the design of high yield catalysts.





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Game Theory Approach for Interactive Wind Farm Control

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Wind energy is widely becoming recognized as one of the most cost-efficient sources of renewable energy. Accordingly, expectations for wind energy are at unprecedented levels as the overarching goal is for wind energy to become a dominant source for global electricity needs. One of the keys to realizing high penetration of wind in a cost-efficient manner is to utilize existing wind farms in a more efficient manner through improved control paradigm.

Most of the existing research on the control of wind turbines focuses on the single-turbine setting. The control of an array of turbines in a wind farm is fundamentally more challenging than controlling a single turbine because of the aerodynamic interactions among the turbines which render most of these single-turbine control algorithms highly inefficient for optimizing power capture in wind farms. One approach for dealing with wind farms aerodynamic interactions is to develop a rigorous model of wake and turbulence for use in distributed control algorithms. However, the variable and chaotic nature of wind makes such a task incredibly challenging. An alternative approach, and the goal of this presentation, is to develop a real time control algorithm where each turbine adjusts its own axial induction factor in response to local information, such as the individual turbine's power generation, local wind conditions, or minimal information regarding neighboring turbines. The axial induction factor is a measure of the decrease in axial air velocity through the turbine and is related to the power the wind turbine extracts from the wind. Here, the goal is to develop a control algorithm that permits the set of turbines to reach a desirable set of axial induction factors that lead to good system level behavior, e.g., power maximization or load minimization, without the need for explicitly modeling the wind.

The field of game theory provides an analytical framework for analyzing systems comprised of enmeshed decision-makers. In terms of wind farms, the decision makers represent the individual turbines and the enmeshment follows from the fact that the decision of one turbine impacts the wind conditions and potential power generation by other turbines. The game theoretic framework is broad enough to model several phenomena that are relevant to wind farms including multiple and heterogeneous decision makers (e.g., turbines with variations in blade size), limited information in decision making (e.g., each turbine has limited information regarding the environment), environmental uncertainties (e.g., variability in wind conditions).

The focus of this exposition is to propose the model free methodology based on game theoretic framework to control and operate the wind farm to attain the optimum equilibrium of the wind farm due to the wake and turbulence within the farm.

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Smart Wind Turbine Rotor Blades

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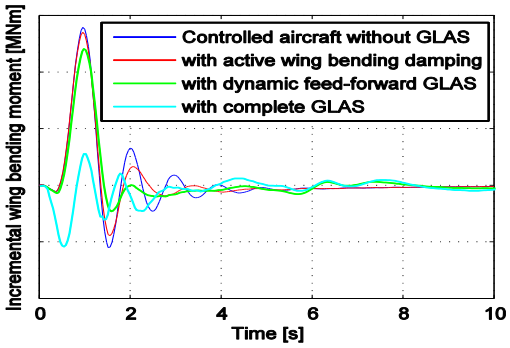
The dynamic response of large rotor blades in rotating machinery, such as in wind energy plants, is strongly interacting with the surrounding unsteady air flow. An in-depth knowledge of these fluid-structure interaction phenomena can help the rotor blade designer to achieve high efficiency and sufficient operational life. The predictions also have to allow for a design offering the required safety on catastrophic failures and aeroelastic instability phenomena like flutter.

In addition to the steady and unsteady flow around the blades, the structural dynamics are also influenced by transient gust loads which might induce additional and undesirable distortions and strains. Since such phenomena are similar to those in aeronautical fixed wings and rotary blades, the approaches and techniques investigated for such aeronautical systems can be transferred to wind rotor blades design. For example, smart blades with proper aeroelastic tailoring and dynamic (gust) load control shall be presented and discussed here. These smart blades shall achieve even higher efficiency and longer operational life of wind energy rotors. For that purpose, different methods and techniques are to be synthesized. These are based on aero-elastic simulation, combined with mathematical design optimization techniques, as well as on active and morphing structures.

Modeling and simulating the aero-elastic behavior by proper coupling of structural and fluid dynamics is an important baseline for the use of optimization techniques for determining proper blade design. Composite materials are an obvious choice, as their properties can be tailored to meet these requirements via variation of the number of plies and the fiber orientation.

In order to additionally control the blade's operational behavior, active dynamic load control methods are investigated based on the concept of active and morphing structures. These induce dynamic trailing edge deformations which may decrease aerodynamic loading and thus overall deflection of the blade. A comparison will be made with active trailing edges investigated for helicopter rotors, where simulation results have been correlated also with experimental results. In case such trailing edge or "rudder" movements have to be larger, this then calls for shape morphing trailing edges where larger distortions or rudder angles are to be induced by proper synthesis of actuators together with proper structural and material properties of such morphing parts. For example, the skin or surface material has to be sufficiently flexible in order to allow high strains but at the same time stiff enough enough to take the resulting aerodynamic loads. Related design and material options for this will be discussed.

Load distribution during a transient aero-servo-elastic simulation of a 5MW class wind turbine



Reduction of aircraft wing bending moment by gust load alleviation
Similar approaches can be applied to wind turbine blades

Early Building Design: Heating and Cooling Plant Approach the Architect

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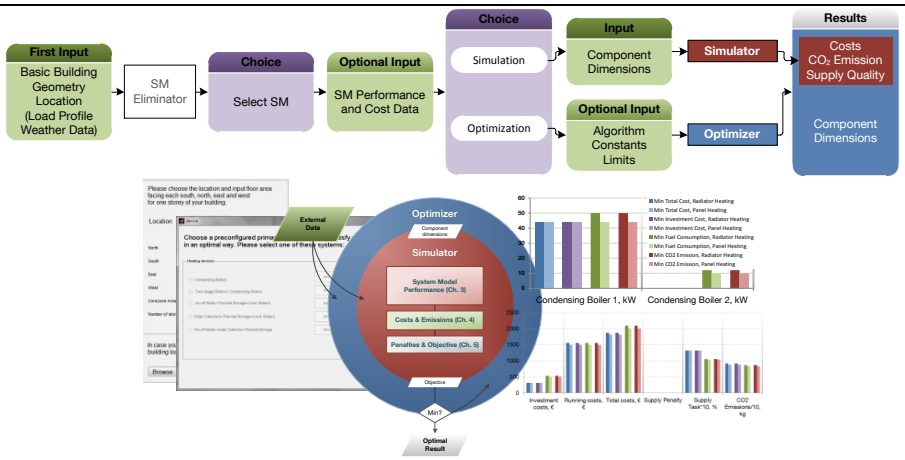
Since heating, cooling and air conditioning (HVAC) of buildings accounts for around 20% of German primary energy consumption, there is a significant reduction potential in this domain. To accomplish this, the design of building energy performance (BEP) is to be pushed towards the very beginning of the conceptual building design process. BEP improves by reducing the building energy demand (e.g. façade design, orientation), increasing the efficiency of energy supply (e.g. distribution system, control, components), and adapting the utilized energy source - including renewable energy sources (RES). Here we propose a tool that helps including the primary HVAC (energy generation plant) into conceptual design.

Although today the efficiency of conventional components such as boilers or chillers is high, further savings can be achieved if utilizing intermittent RES, thermal storage and good controls. Since some of the components impose restrictions on building design and can later not be introduced, the BEP benefits from the architect knowing what energy source to account for right from the beginning. To enable this we developed a primary HVAC simulation tool capable of:

- Implementing intermittent RES and thermal storage by using time domain simulation;
- Optimal boiler and chiller staging considering part load efficiency;
- Component size optimization (goals: total or investment cost, carbon emission and fuel consumption minimization);
- User interface suitable for non-experts and reduced user input data demand suitable for conceptual design.

After guiding the user through a clear set of steps the tool provides dimensions, annual costs, energy consumption and emissions of the optimized system. Comparing alternative designs leads to early recognition of environmental or/and financial benefits of certain systems. Such an approach is gaining importance with the increased utilization of complex hybrid systems, due to the difficulty in experience-based initial dimensioning.

Each building represents a dynamic object in the energy map of the area it is located in. Apart from aiding the early design, the simulation tool can perform energy analysis of the existing building stock or help planning multiple buildings.



System modeling for energy-efficient and sustainable building design and city planning

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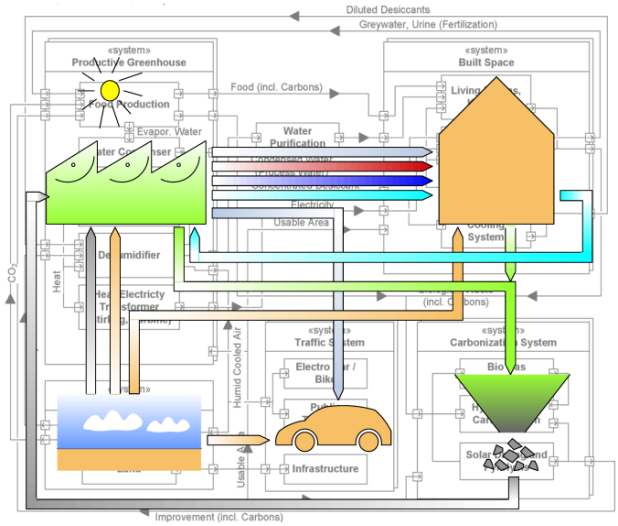
To achieve energy-efficient sustainable design solutions for cities and buildings is a highly complex and interdisciplinary task. Current design practice proceeds in a mainly sequential way neglecting complex interdependencies, e.g. between energy efficiency, environmental and economic resource consumption. Due to this neglect the full potential of efficiency is not exploited. Furthermore, the integration of renewable energy technologies requires a careful coordination of the components. Therefore, the presented research approach develops a method of systems modeling for urban and building design to represent these complex dependencies that are necessary to consider for achieving efficient and sustainable design solutions. The approach establishes a systems model for the building domain that interacts with the geometry-focused modeling, which currently dominates building design. The system model is able to complement these models by the key engineering interdependencies and their explicit modeling for innovative solutions, e.g., in terms of energy management. The approach uses the Systems Modeling Language (SysML) as a current state-of-the-art modeling language of systems engineering and adopts it for the building domain. The process of systems modeling based on this language starts from the early phases of design by capturing the use and the respective requirements of the system; it continues to final result of a system model, which are system flow diagrams and performance-oriented parametric diagrams. Two examples from urban and building design serve to illustrate the use of systems modeling for performance-oriented design for energy-efficiency and sustainability. The first example outlines by simple considerations the setup of a CO2-absorbing city based on greenhouses, electric vehicles and a desiccant-based heating system for buildings. The second example shows a system-based strategy for the interaction of quantities and qualities in the ongoing research project Nuremberg Weststadt, which aims at a sustainable and livable city district, in order to link technical sustainability, e.g., energy efficiency, with the qualitative descriptions of the livable city.



Smart Grid Demonstrator of a Future Office Prosumer

Denis Bytschkow[a], Pragya Gupta[b], Dagmar Koss[c], Steffen Bauereiß[d], Florian Sellmayr[e], Bernhard Schätz[f]

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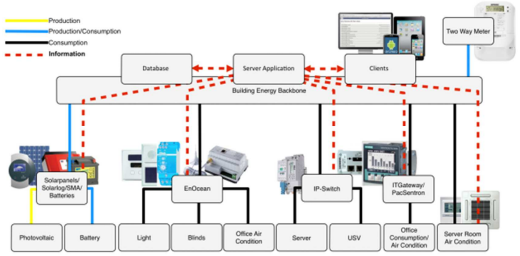
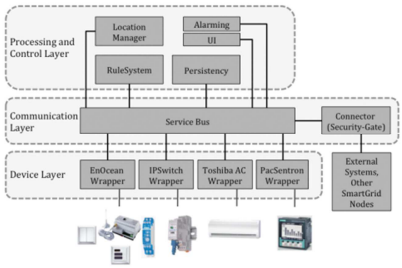
The increasing integration of renewable energy from private households and companies, which are connected to the medium and low voltage level, starts to change our energy system drastically. New challenges in the energy system not only include the balancing of volatile, largely distributed, small-volume energy production and consumption, but also a shift of centralized overall control infrastructure to more localized and decentralized approaches. This requires new smart energy systems, which will support the management of available energy production and distribution on the local level.

This work focuses on establishing new system architectures and their implementation in form of a hardware and software demonstrator – as a *Living Lab* in everyday use – for distributed energy systems, forming an intelligent node in a smart grid infrastructure environment. The developed smart grid node includes energy consumers, producers, buffers, sensors, actuators and ICT components. In order to achieve core smart grid requirements like easy integration of heterogeneous electrical devices by plug and play capabilities, scalability, distributable, robustness and self-recovery, the developed smart node architecture is designed for maximal flexibility. Besides the control of heterogeneous devices, the architecture covers integration of sensors and actuators to enable control mechanisms for energy efficiency and to support a wide variety of advanced application scenarios like peak shaving, providing a demonstrator to evaluate the applicability of the architecture for smart energy systems.

The Living Lab integrates several devices into an office space environment, such as smart meters, home automation units, solar panels, batteries, air-conditioner etc. The smart node enables metering/monitoring, storing, processing, and analyzing the status and data of individual devices, aggregating it into the status of the overall smart grid node. The control logic of the demonstrator includes methods to decide on and perform actions to achieve better energy efficiency (e.g., turning off unused lights or control the air conditioner). Besides basic energy saving the *Living Lab* can also be used to demonstrate methods, which are currently investigated in the smart home research community. This includes optimization and control of appliances (like dish washer, refrigerator, smart home devices etc.), which can operate at times when the energy prices are lower. By rescheduling loads, smoothing energy peaks, and communicating available loads and capacities with the external smart grid, the demonstrator shows how combined control and configuration algorithms of several nodes can help to increase the reliability and stability of the power grid.






```
rule "Simple AC/Temp Example"
when
//Check for events
   DoubleEvent(
      $val: value,
      "Celsius",
      $org : origin
      ),
   $val: 25.0;
then
//issue command for every device associated
//with the events origin
for (Device d :
   locationManager.getAssociatedDevices($org)){
   if (d.devType == "AC"){
   //Turn ON command issued here
   commandUtil.setBoolean(true, d);
   }
}
end
```

3 Poster Presentations

Pretreatments for Bioenergy Use of Egyptian Rice Straw

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The world is suffering from problems of climate change caused mostly from the use of fossil fuels. At the last decade, many countries have turned to the essential crops for biofuel production. However, biofuel crops created many problems due to the loss of food crops and therefore gaps in feed requirements especially in most of undeveloped countries. Many challenges are focused on using farm waste products for biofuel production instead of essential crops.

Based on literature studies rice straw was selected as a most abundant lignocellulosic waste in the world. Especially Egypt is the largest rice producer in the Near East region producing 7.25 million tons rice / year leaving about 4.96 million tons straw / year in the fields as a crop residue. The farmers use about (20%) of the rice straw and about 3 million tons are burnt by farmers in the field. The resulting emissions of CO_2, CO, CH_4, NMHCs, NOx, NH_3, N_2O, SO_2 and other particulate and trace gases from open burning of rice straw cause air pollution in form of the “Black Cloud”. Alternatively, it can play an important role in Egypt's economy in the future when we use the straw to produce biofuel beside other beneficial products. This would reduce the air pollutions from burning the straw and reduce the use of petroleum hydrocarbons as an unfriendly environmental fuel, which would lead to decrease the loss in food crops.

The challenge for the use of the rice straw potential is the complex structure of cellulose, hemicellulose, lignin, silica and wax that make a barrier for the digestion of the straw. For this, our research aims to the production of environmental friendly biofuel in addition to other organic products of high economic value by different methods of pretreatment of Egyptian rice straw to convert the polysaccharide chains structure to fermentable sugars without or with low levels of inhibitory compounds and at low costs.

Rice straw samples were collected and transported from Egypt to Germany, then washed, dried and milled to 1-2 mm to be ready for further analysis and treatments. After evaluation of the physico/chemicals and microbiological properties to create a full overview on the Egyptian rice straw, several pretreatment methods and conditions were selected for pretreatment tests as most efficient methods according to literature: lime, urea, microwave/dilute acid, alkaline peroxide with different type of alkaline (NaOH, $Ca(OH)_2$ and CH_4N_2O). We used the central composite Design based response surface for 3 factors for the optimization of experimental parameters (concentrations, temperature and time). Then we hydrolyzed it using two different commercial saccharolytic enzyme preparations.

The main components of carbohydrates found in rice straw were glucose (39.24% w/w of dry mass) and xylose (26.40% w/w of dry mass). Arabinose and galactose were less than 1-2 % of the rice straw dray mass.

The NaOH - H_2O_2 pretreatment turned out to be the best of the tested methods with an efficiency of saccharide recovery of around 97 % after pretreatment and enzymatic saccharification. Alkaline peroxide pretreatment in combination with enzymatic saccharification can almost completely convert the polysaccharide chains structure of rice straw to fermentable sugars without inhibitory compounds and the generated hydrolyzate can be fermented to produce valuable substances, e.g. bioalcohol, fats or microbial polysaccharides.

Keywords: Egyptian rice straw, pretreatment, enzymatic saccharification

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Analyzing the Environmental Performance of Induced, Operational, and Embodied Impacts of Buildings

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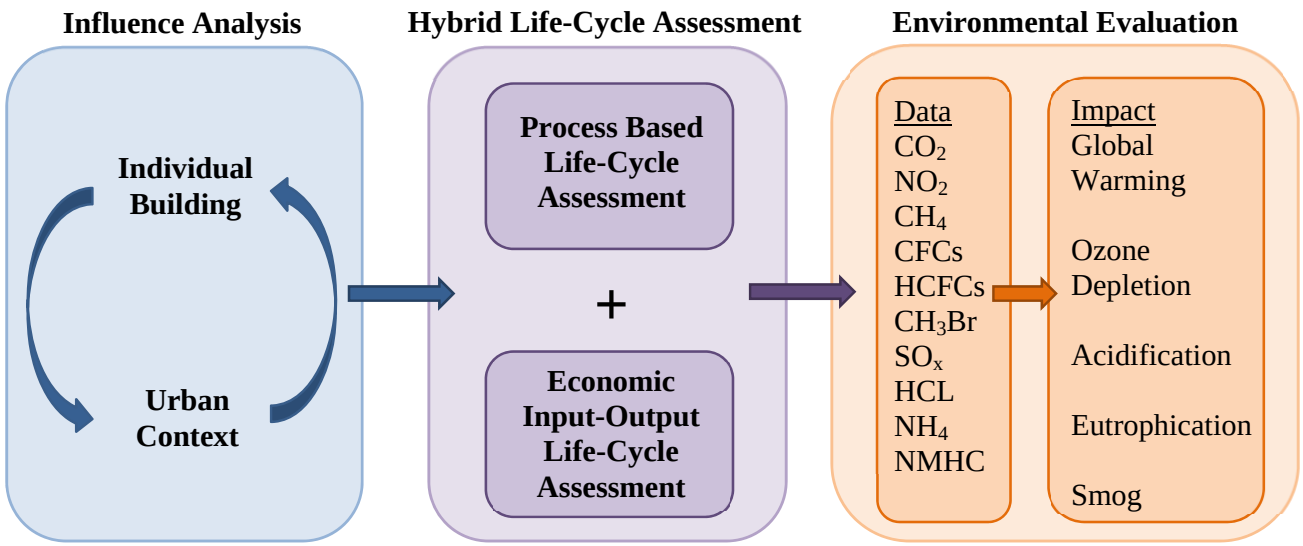
Mitigation of, and adaptation to, climate change is intimately dependent on the role of the urban environment. Research and practical applications of environmental design focus primarily on the energy-efficiency of buildings. Studies have shown that in multiple-building settlements, mobility and lifestyle choices are of significance in energy consumption in addition to the traditional environmental impact categories of embodied and operational energy. However, in existing cities the construction of settlements is infrequent compared to individual building construction due to limited space within the dense urban fabric. Consequently, the paper presents research on a new metric, induced impacts, and the methodology to account for the environmental impacts accruing from the interactions of an individual building and its surrounding urban context.

Understanding the interface of an individual building within the larger urban environment is crucial in achieving sustainability objectives. The paper presents new research on the environmental impacts resulting from the bottom-up interaction of buildings within cities focusing on mobility, the influence of mixed-use construction, daily interactions (e.g. shopping, school/work), and other factors in the larger urban experience. The research quantifies the impact categories for various locations within a major Central European city. The induced impacts, in addition to operational and embodied impacts, will be evaluated utilizing life-cycle assessment methodologies to quantify the environmental effects. In order to expand the results beyond ubiquitous energy consumption, the research is based on life-cycle inventory data, thereby illustrating potential environmental trade-offs. The results of the investigation will show the potential for planning strategies to optimize the environmental performance of urban areas through focused attention on induced impacts in addition to operational and embodied impacts. The research is highly relevant for designers, planners, and building-code and rating system administrators in achieving environmental sustainability objectives.



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A flexible aerodynamic surface as innovative design for an adaptive wind turbine blade

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The reduction of greenhouse gas emissions is a central problem of the modern society, and the increasing ecological awareness drives the development of sustainable energy supply. In this context, wind turbines certainly play an important role as well established zero-emission power plants. Thanks to modern designing tools and production techniques, state-of-the-art wind turbines reach very high efficiency at design operation point. However, the drastic drop in performances at off-design conditions, for example due to varying wind speeds, remains an inherent problem associated with the classical rigid blade construction. In order to address this problem, alternative blade designs using adaptive structures based on compliant materials could be considered, thus allowing more efficient and flexible wind based energy production.

In this context, ongoing investigations carried out at the Institute of Aerodynamics and Fluid Mechanics of the Technische Universität München focus on the development and analysis of such an adaptive aerodynamic surface. Primarily developed as an innovative high efficient airplane wing, the concept shows features that could be taken advantage of for a novel wind turbine design as well. The basic construction of this morphing membrane wing uses an articulating, load-bearing frame structure over which a compliant membrane is spanned to form the actual aerodynamic surface. Due to its high flexibility, the membrane significantly deforms under aerodynamic load and, as a result, its shape naturally adapts to varying operating conditions. This behaviour provides the wing with a passive flow control mechanism, which is likely to alleviate structural loads due to gusts or stall. In addition, the non-linear aerodynamic characteristics result in increased lift production that can be used to adjust the absorption of wind energy depending on the operating conditions.

The presentation will provide more details about the specific characteristics of this adaptive wing and discuss a potential application as an innovative blade for wind turbine.

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FHI-aims becomes embedded: full-potential QM/MM approach

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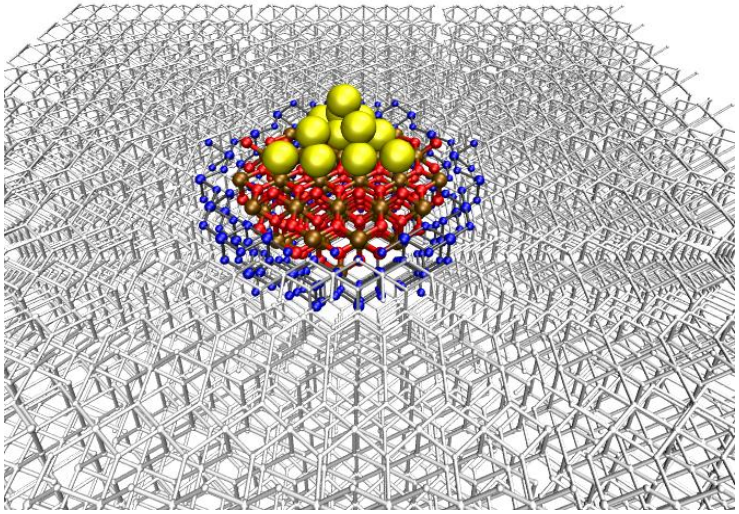
Noble metal nanoclusters are receiving increased interest for their ability to support the photoinduced splitting of water at semiconducting surfaces. In comparison to their bulk counterparts nanoclusters in the none-scalable size regime are suggested to act either as potential chromophore and/or provide special active sites for the surface chemical reactions.
In order to address these functionalities through quantitative first-principles calculations a computationally most efficient description of possibly locally charged semiconducting systems is required. Properly accounting for long-range electrostatics without getting troubled with spurious interactions with periodic images, embedded cluster models are an appealing option to this end. Here, we present a corresponding implementation for the full-potential FHI-aims package. In order to prevent electron leakage into the Coulomb singularities, we describe the linking atoms at the QM/MM-boundary at the level of norm-conserving pseudopotentials. The fully separable form of the employed Kleinman-Bylander pseudopotentials allows for fast evaluation of the interaction integrals, especially in combination with FHI-aims' efficient atom-centered basis sets. We demonstrate the high accuracy and computational efficiency of this approach with applications to TiO_2(110)-supported gold clusters.



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Backing up renewable energy supply – responsible power generation with fossil fuels

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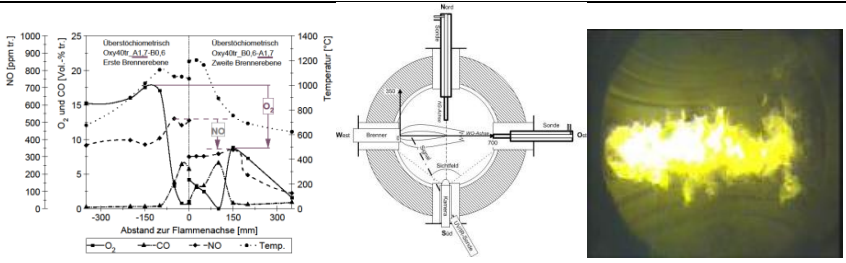
Under the impression of the Fukushima accident and based on a consensus by a broad majority of policy makers and the general public, Germany has decided to opt out of nuclear energy generation by the year 2022. Even before this agreement was reached the annual growth rate of renewable energy production in Germany was high compared to countries with comparable electricity generation systems. While the nuclear phase out is even pronouncing the trend to an increased share of “green electricity” in the transmission grid, efforts to adapt the infrastructure to new challenges imposed by this trend are lacking behind drastically. Renewable energy sources such as wind and solar power are characterized by its volatility due to day/night and weather shifts. The infrastructure of a grid dominated by renewable energy sources has therefore be designed to be able to compensate for load shifts triggered by volatility in demand and generation. Apart from new transmission routes to connect large generation sites in the north of Germany with the south a modern power generation system has to incorporate large capacity storages as well as back-up production sites which qua definition are not dependent on wind and sunshine.

Back-up electricity production has to feature certain design characteristics. While having a steep start-up ramp (quick-start-ability), the amount of available power has to be relatively large in order to replace generation capacity from wind or sun in a large scale if needed. For the purpose of quick start-up gas fired power plants or combined cycles are considered most promising. When it also comes to the price of production (medium term back-up) coal fired power plants feature a compromise between start-up characteristics and production cost.

Common to both technologies is the high emission level of CO2. Research is being done worldwide to reduce the relative emissions ([kg-emissions/MJ-electricity output]) of fossil fired power plants by either increasing the plant efficiency or sequestrating and storing the CO2.

At the institute for energy systems in the frame work of an EU co-funded project oxyfuel coal combustion is being investigated experimentally as a means to generate electricity from coal while limiting carbon dioxide emissions to only a few percentage points of comparable power plants without sequestration. In a coal fired combustion test rig with 200kW thermal power different burner concepts and different firing strategies are being compared in terms of overall efficiency and process handling. Optimal operation windows are to be determined in the process. All experiments are accompanied by CFD simulations in order validate models and vice versa to reduce to amount of measurement point. First results are expected for late summer.



A model-predictive energy management for a home energy system based on a genetic algorithm

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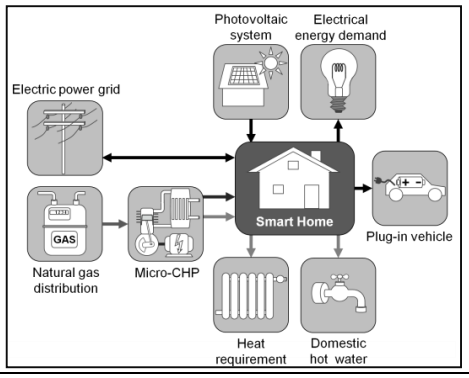
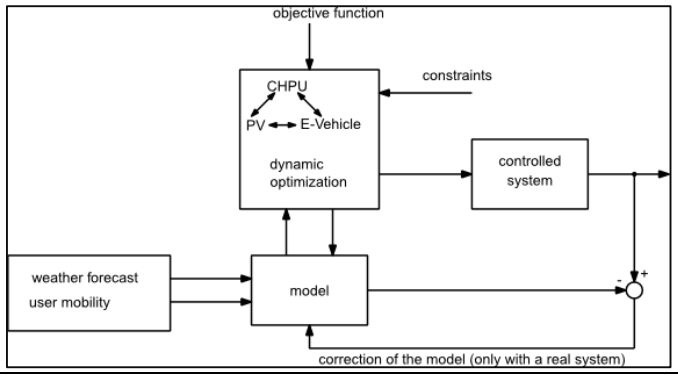
In current research projects such as "vehicle to grid" (V2G), "Vehicle-to-Building" (V2B) or the "Smart Home" plug-in vehicles are integrated into stationary energy systems. Thereby, Smart Home or V2B stands for an intelligent networking between vehicles and buildings. Whereas in this regard the most efforts are limited to smooth the electrical load profile on a household level through optimized charging and discharging of electric vehicles, in this paper such a small decentralized energy system consisting of a building and vehicle is investigated from a holistic point of view. Thermal as well as electrical system components are taken into account and the reduction of the overall energy consumption and the CO2 emissions will be focused.

A predictive energy management is presented that coordinates the energy system components of a building and the system integration of a plug-in hybrid vehicle and optimizes the system operation in terms of energy consumption and CO2 emissions. Therefore, a model predictive control (MPC) approach is applied on the energy management of a "smart home" with integrated power generation by a cogeneration unit, a photovoltaic system as well as on the charging phases of a plug-in hybrid vehicle. The energy management system contains, similar to a MPC controller, a model of the system dynamics. With this model a prediction of the energy process is conducted based on a weather forecast for three consecutive days and future mobility patterns. Thus, the future development of all relevant variables is predicted. Based on this prediction, a dynamic optimization of the operational management takes place. As part of this prediction process the best strategy for the manipulation of variables is determined and selected. Therefore, a genetic optimization algorithm is used in a way that ensures the desired course of the state variables. From the sequence of future control variables which are calculated in the current time step, the first element is passed to the process. Then, the time horizon slides forward by a sampling step and the entire sequence consisting of prediction and optimization run through again.

Thus, for the energy management of the small energy system an approach similarly to the model-based predictive control is proposed which includes the elements of prediction, dynamic optimization and the principle of the moving horizon. The energy management system optimizes and coordinates the use of components and the energy flows within the coupled energy system. Involving the entire "Well-to-wheel" chain this enables on the one hand an ecological system operation and a cost-effective one on the other.





Energy conversion & storage: fundamental insights in batteries and fuel cells

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In order to improve the performance of energy storage and energy conversion devices significantly, new approaches have to be explored. Developing new materials and morphologies based in part on principles observed in nature is our strategy to address the challenges in energy research.

A major disadvantage of carbon supports, which are used in many commercial catalyst systems, is that they are prone to corrosion. Titania is more corrosion resistant compared to carbon and hence a promising material for medium and high temperature applications, such as the direct conversion of ethanol in proton exchange membrane fuel cells (PEMFC). However, the application of titania in electrocatalysis is limited due to its poor conductivity. An enhancement in the conductivity can be achieved by a high temperature carbothermal reduction treatment which converts titanium dioxide (TiO_2) into titanium oxycarbide (TiO_xC_y). A detailed investigation of the carbothermal reduction process has been carried out by studying compact anodic TiO_2 films after treatment at different temperatures and a thermodynamic model was proposed [1].

To test the applicability of compact TiO_xC_y as a support material for electrocatalysis, aerosol assisted deposition (AAD) of platinum on compact TiO_xC_y films has been performed and its electrocatalytic activity for alcohol oxidation will be discussed.

A great deal of interest has been developed in the recent past towards enzyme catalysis for energy conversion. In order to obtain a fundamental understanding of oxygen reduction reaction electrocatalysis, investigations of enzymes directly immobilized on electrode surfaces are of great value. A combination of interfacial bioelectrochemistry and scanning probe microscopy provides an excellent tool to investigate the electrochemical activity of redox enzymes on model electrode surfaces as it is capable of in-situ mapping of the direct electron transfer between a single redox molecule and the electrode. Preliminary results of our electrochemical and scanning probe microscopy studies of an oxygen reduction catalysing enzyme, laccase, immobilized on Au(111), are also presented. Analogous investigations on conductive titania substrates are anticipated.

Besides its applications in electrocatalysis, TiO_xC_y is a promising anode material for lithium (Li) ion batteries. The Li intercalation properties of TiO_xC_y strongly depend on its morphology and crystal structure. Nanotubular TiO_2 offers improved Li intercalation because of the enhancement of electrode charge-discharge rates resulting from shorter diffusion paths [2]. Preparation of TiO_2 nanotube arrays, their conversion to stable TiO_xC_y nanotube arrays and their lithium intercalation properties are also discussed in this presentation. Currently studied is the application of nanotubular TiO_xC_y as a conductive support for Si, with Si being a high capacity anode material for Li intercalation.

[1] C. Ruediger, F. Maglia, S. Leonardi, M. Sachsenhauser, I. D. Sharp, O. Paschos, *Electrochim. Acta*, accepted.

[2] A. S. Bruce, B. Scrosati, J. M. Tarascon, W. Van Schalkwijk, *Nat. Mater*. 4 (2005) 366.

Li_6PS_5X (X = Cl, Br, I) - Solid Electrolytes as Diffusion Barriers in Lithium Sulfur Batteries

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Recently, lithium ion battery research has focused on lithium sulfur batteries due to their high theoretical capacity (1675 mAh g_S^{-1}). One of the main challenges is the shuttling of soluble polysulfides during battery cycling from the sulfur positive electrode to the lithium negative electrode. The shuttle mechanism induces loss of active sulfur material from the positive electrode through deposition of Li_2S on the negative electrode, thus resulting in a gradual loss of capacity. To inhibit the polysulfide shuttle, the possible use of solid electrolytes is investigated. Promising candidates for solid electrolytes are the halide lithium argyrodites, Li_6PS_5X (X = Cl, Br, I). According to *Deiseroth*[1], these materials show a high lithium conductivity and they are electrical insulators. Halide containing lithium argyrodites were synthesized and identified by x-ray diffraction (XRD). Stability tests in oxygen and air were performed. Lithium ion conductivity and the stability of these materials towards metallic lithium were measured by impedance spectroscopy. The thermal stability was investigated by thermogravimetric analyses (TGA).

Reference:

[1] H. J. Deiseroth, S. T. Kong, H. Eckert, J. Vannahme, C. Reiner, T. Zaiss, M. Schlosser, *Angewandte Chemie-International Edition* **2008**, 47, 755–758.

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Modeling of ionic liquids as electrolyte for Lithium batteries

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Ionic-liquid-based electrolytes have recently received particular attention for electrochemical storage and conversion applications. This is due to the fact that, compared with conventional liquid-based electrolytes, they offer several advantages. In particular, Ionic Liquids (ILs) provide: i) high chemical and thermal stability, ii) a broad electrochemical stability window, iii) low vapor pressure and iv) non-flammability. Various studies considering ILs can be found but the capacities obtained are still lower than when using carbonate-based electrolytes [1]. However, the advantages of ILs are instrumental in the development of all types of Li-batteries such as Li-ion, Li-S, Li-O_2 batteries. The development of advanced computational methods for simulating electrolytes based on ILs enables important insight into their basic physical and chemical behavior, which cannot be gained otherwise, in general. This presentation will outline our first steps towards developing such a computational method.

Commonly used aprotic electrolytes and ionic-liquid-based electrolytes have to be distinguished. Aprotic electrolytes are binary systems, where the ions from the salt (Li salts) represent the only charge carriers, whereas ILs consist exclusively of ions. Thus, the dilute solution theory is basically restricted to dilute aprotic systems. In contrast, ILs need to be considered on the basis of an appropriate model for concentrated solutions, which is considerably more complex and has not been as thoroughly investigated as the dilute solution theory. Furthermore, the physical properties of ILs, such as diffusion coefficients or transference numbers, significantly differ from the properties measured in dilute electrolytes. It also has to be emphasized that the concentration dependence of these properties may not be negligible anymore, as it is usually assumed for electrolytes based on the dilute solution theory.

The transport equation for reacting species in a binary electrolyte assuming dilute solution theory, electroneutrality, and the absence of notable volume changes during battery cycling can be written as

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - D_{\text{eff}} \Delta c = 0; \qquad (1)$$

see, e.g., [2]. In this equation, ion transport due to migration is included in an effective diffusion coefficient D_{eff}. For such systems, the effective diffusion coefficient, which is only marginally depending on the concentration, can be easily determined by measuring the limiting current density.

In electrolytes based on ILs, ionic interactions, according to the concentrated solution theory (see, e.g., [2] and [3]), need to be taken into account. As an initial step, the applicability of equation (1) for binary as well as for tertiary ILs is investigated. For this purpose, the effective diffusion coefficient is determined as for a system with aprotic electrolyte. The quality of the numerical results based on equation (1) and the determined constant effective diffusion coefficient D_{eff} is evaluated on the basis of experimental data.

[1] A. Garsuch, D. M. Badine, K. Leitner, L. H. S. Gasparotto, N. Borisenko, F. Endres, M. Vracar, J. Janek, R. Oesten, Investigation of various liquids and catalyst materials for Lithium-Oxygen batteries, Zeitschrift für Physikalische Chemie 2012, 226 (2012) 107-119.

[2] J. Newman, K.E. Thomas-Alyea, Electrochemical Systems (3rd edition), John Wiley & Sons, 2004.

[3] R. Pollard, J. Newman, Mathematical modeling of the Lithium-Aluminium, Iron Sulfid Battery: I. Galvanostatic discharge behavior, Journal of the Electrochemical Society 128 (1981) 491-502.

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Sustainable building performance monitoring with adaptive energy control

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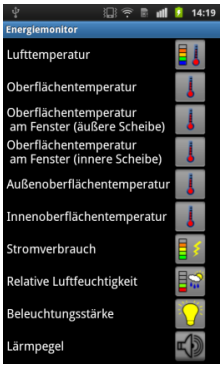
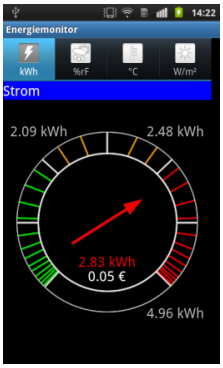
The suitable preparation of energy data for the consumers of energy is an important factor for energy saving. Energy monitor systems on smartphones can support the user with the right information at the right time. First we analyzed two projects which are state of the art, the IBM TIRIGRA[1], and the Allnet Home automation[2] project. The aim was to generate a basis for collecting and analyzing energy data on demand. Therefore a prototype for an energy monitor system was implemented as a smartphone application. The system is able to 'know' about its environment. This implies to measure additional data e.g. weather data especially from the broader surroundings to offer services that will keep the users in a comfort climate. Another feature is the knowledge of the position of joint users, which needs a rule and multiuser management. For this the system architecture is divided into three parts the testing environmental (measurement), the web service environmental (data preparation), and the energy monitor environment (displaying, view). To manage the data flow in between the environments and not to consume lots of energy the structure of data (XML-Document, JSON-Object), the range of updates are important factors. To provide the users with helpful information, different types of views are implemented. The first control surface shows the users an overview of his consumption in identified areas (test environment). This generates an on demand feedback of the energy consumption for the users. Furthermore the users are informed by services via signals which could be haptic, acoustic, or visual. This enables the users to manually or automatically react on demand on significant changes in the energy consumption. Reacting on events can be done manually in the device control view. The energy monitor systems provides the user with more security[3]. The safety aspect is observed by the user management e.g. username, and password and encryption algorithm for the transfer of data. Future work is creating profiles and predictions to provide the users with data when he can reduce consumption or should store energy.

References

1. IBM Corporation, *Enterprise Asset- und Service Management. IBM Intelligent Buildings Management TRIRIGA CAFM/IWMS*, 2012: Hannover.
2. ALLNET. *Home automation*. 2012; Accesed 17.04.2012; Available from: http//www.allnet.de.
3. EnBW. *Smart Metering: Der intelligente Stromzähler*. 2012; Accesed 20.03.2012; Available from: http://www.enbw.com/content/de/magazin/energiespartipps/energiespartipps_stromverbrauch_im_blick/index.jsp;jsessionid=BA4F020BABA243711C55EC101840FB87.nbw05.



Main view [Gottlieb M. 2012]



Detailed view [Gottlieb M. 2012]

Device control view [Gottlieb M. 2012]

Formal Smart Energy System Engineering Method

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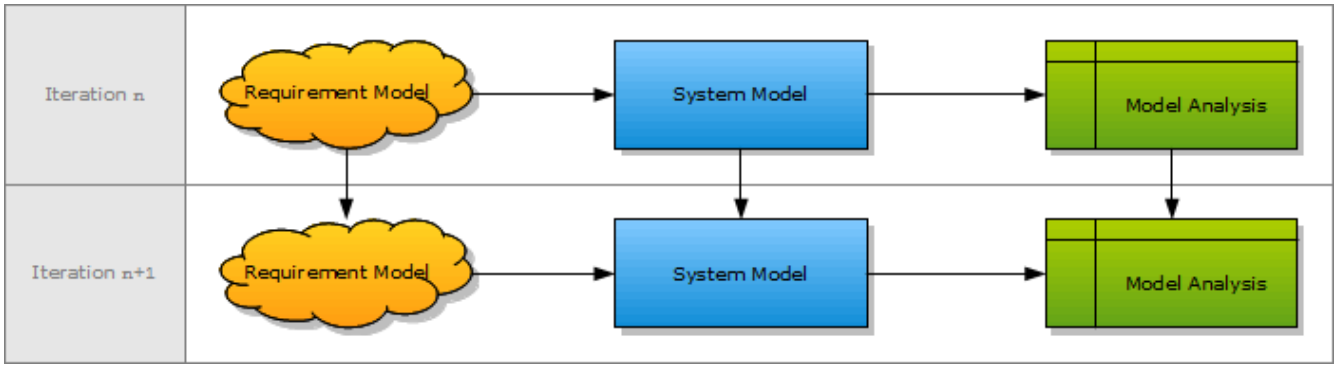
The energy turnaround imposes new requirements on the energy system and consequently new challenges on energy system engineering. New requirements are for example the transition from fossil to renewable energy sources, decentralized energy production and increased energy efficiency. These requirements are complemented by existing requirements regarding reliability and scalability of the system. ICT is broadly accepted as one major piece of the engineering puzzle. However, the concrete architecture, design and implementation are under heavy discussion. The design options are plenty and the design space is vast leading to numerous different approaches.

To improve ICT engineering we propose a method, which is based on experience in the automotive and avionic domains, where critical safety requirements demand extensive testing for software components to be certified. This is why over the years formal engineering methods have been introduced, which promote systematic and seamless model-based engineering from high-level requirements to implementations. An iterative top-down approach allows early testing of requirements on coarse system abstractions while enabling continuous refinement. Overall, the engineering paradigm leads to better solutions in shorter time due to decision support in all project phases.

Applying these ideas to the energy domain means finding suitable abstractions for modeling both the requirements and the system components, while obtaining useful results from model analysis for guiding the iterations. Currently, we focus on sums of active power for calculating the balance between produced and consumed energy inside households and across voltage levels neglecting reactive power, voltage, frequency and other physical properties. Hereby, power is expressed as a number with the sign indicating the flow direction. Consequently, the electric system is modeled as a tree of electric components each generating an observable energy output with the respective flow direction. Finally, to introduce smartness the electric system is connected to a control system. The control system is responsible for processing sensor measurements and generating commands for the electric components.

Having this coarse model of the “ICT-enhanced” energy system the smart grid engineering challenge is formulated as the challenge to specify a control system behavior that satisfies all relevant system requirements. In particular, in early phases we investigate core requirements such as power balance and consumer priority (e.g. hospital over household). In later stages requirements such as energy or cost efficiency can be added.

In the future we plan to extend the model of the electric system to express more realistic behavior, develop formalisms to model dynamic system structures (e.g. for electric cars), tune the method towards developing optimization algorithms, and investigate usability in interdisciplinary settings.



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Economic potential through ecological efficiency in the building sector accounting for social and global perspectives regarding feedback loops

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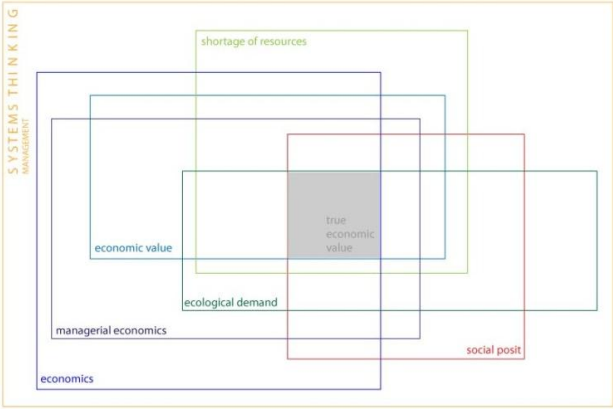
Entrepreneurship is challenged by increasing demand and rising world-market prices for resources. Environmental and life-cycle costs, recycling possibilities, as well as influences on society are aspects, which have to be measured during the entire product life-cycle. These interdependencies have to be taken into consideration for a qualitative decision to be made on the design of products and processes. Therefore, comparable information is required. High-quality information concerning resource consumption, resources management and possibilities for resource reduction has to be provided. “Sustainable development” is seen as a dynamic concept, a principle of a regulative idea based on diverse time-frames, scales and space, which should influence management decisions. This complexity requires systems thinking.

This work aims to illustrate the interrelation between economic value and resource efficiency, without loss of quality (i.e. functionality, social value, and aesthetics). The research fills the information gap on indirect resource flows of processes and products on a global level, focusing on management decision-making in order to achieve sustainable development. Further, the economic value of materials in the global economy must account for international background, social justice, and limited resource availability.

Value chains of wood, steel, glass, and cement are investigated concerning production, refinement, and consumption. CSR and GRI aspects (e.g. sustainable society index, sustainable value working environment, employment, human rights, social sustainability (SIA 112/1)) are taken into consideration as social aspects. Changes of ecosystems within the resource extraction are mentioned by the example of phosphor loss as an indicator for environmental performance as also grey and primary energy consumption. Medium-sized enterprises are examined. Economic performance is measured based on life-cycle, economic value, willingness to pay, total cost of ownership, and product quality.



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Efficient electricity generation from renewable sources with Solid Oxide Fuel Cells

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The EU-JTI project SOFCOM is aiming towards the demonstration of electricity generation from biogas and gasified biomass using Solid Oxide Fuel Cells (SOFCs). These provide several advantages over more conservative concepts like gas engines, especially higher overall system efficiency.

However, especially direct coupling of SOFCs to biomass gasification systems is critical due to pollutant formation during the gasification process. Within the project, the impact of several types of pollutants (e.g. sulfur, tars) and relevant cleaning strategies are being investigated. At TUM, research is focused on the impact of tars on SOFC anodes. External and internal tar reforming are being studied to ensure safe long-term operation of the SOFCs.

Parallel to lab-scale experiments on SOFC anodes, theoretical modeling of efficient Combined Cooling, Heat and Power (CCHP) plants with varying system components (e.g. different gasifiers), as well as two demonstration plants in Italy and Finland are used for techno-economic evaluation of the whole concept.

In a final step, during the demonstration phase CO2 sequestration from oxy-combusted SOFC exhaust is being investigated. Here TUM is responsible for design and construction of the device.

Within a future European energy network, the feasibility of providing CO2-neutral, highly efficient small to medium-sized power plants for independent electricity generation from locally available renewable sources will help achieving climate protection goals, as well as providing a reliable source of energy for small, rural communities.

PhotoCOO:A collaborative research project investigating the photocatalytic CO2 activation

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The photocatalytic conversion of CO_2 into fuels is a prerequisite for a closed, carbon based energy cycle and it can be an important contribution to an energy supply mainly based on renewable energies. In the BMBF supported collaborative research project „PhotoCOO“ five groups from the chemistry and physics departments of the TUM and the Südchemie AG jointly develop scalable concepts for the photocatalyic, water based conversion of CO_2 to fuels and basis chemicals, such as ethane, methanol or formaldehyde, employing both, homogeneous and heterogeneous catalysts. PhotoCOO is part of the upper level cluster project iC4: Integrated Carbon Capture Conversion and Cycling cluster. In our contribution, we will introduce the aims of PhotoCOO, and discuss one CO_2 conversion route, the photoelectrochemical reduction of CO_2 at p-Si electrodes modified with catalytically active organic molecules, in more detail.

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Nanotubular TiO_2 – 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_2 on Ti [2,3] is among the most promising structures since it offers several interesting functional properties.

The growth of self-organized TiO_2 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_2 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 ~ 1.1µm to ~ 3.2 µm.

References

[1] H. Masuda, K. Fukuda, Science, **268** (1995) 1644.
[2] V. Zwilling, M. Aucouturier, E. Darque-Ceretti, Electrochim. Acta, **45** (1999) 921.
[3] J.M. Macak, H. Tsuchiya, A. Ghicov, K. Yasuda, R. Hahn, S. Bauer, P. Schmuki, Curr. Op. Solid State Mat. Sci., **11** (2007) 3.
[4] R. Hahn, F. Schmidt-Stein, J. Salonen, S. Thiemann, Y.Y. Song, J. Kunze, V.-L. Lehto, P. Schmuki, Angewandte Chemie Int. Ed. (VIP Paper), **48** (2009) 7236.

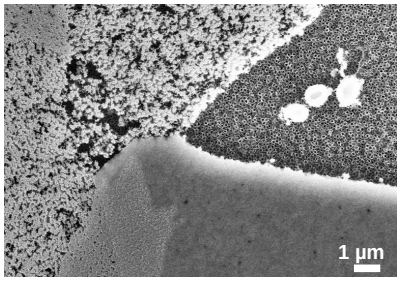

Fig. 1: TiO_2 nanotube growth depends on the grain structure.

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Eulerian two-fluid simulation of immersed tube erosion in fluidized bed combustors

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Fluidized bed combustion (FBC) is widely applied for energy production. It offers several advantages over the conventional combustion techniques with respect to its high fuel flexibility and low pollutant emissions. One persistent problem in FBC is the accelerated wastage of the heat exchanger tube surfaces. The wastage caused by erosion may cause the immersed tubes to burst, and this issue would affect the economics and safety of the power plant [1,2]. In this work the erosion process was simulated in a bubbling fluidized bed equipped with a dense tube configuration using the two-fluid model.

The experimental work of a bubbling fluidized bed was conducted by Johansson et al.[3] and the in-bed hydrodynamics and erosion were simulated using the Eulerian two-fluid model coupled with the monolayer kinetic energy dissipation model developed by Lyczkowski et al. [2]. The open source CFD software OpenFOAM [4] was adopted to simulate the hydrodynamics in the gas-solid flow system. The original OpenFOAM solver named as twoPhaseEulerFoam was modified and extended to simulate the particle volume fraction, gas and solid phase velocities and the erosion rates around a target tube.

The simulated erosion rates were compared with the experimental data as shown in Figure 1. Although there is room for improving the fluid dynamics and erosion models, the qualitative agreement was acceptable taking into account the complex hydrodynamics and the uncertainty of the measurement.

The hydrodynamics in the fluidized bed was described by the solid volume fraction and gas velocity as shown in Figure 2. The dense tube distribution broke the large bubbles into small ones, which would greatly enhance the gas-solid mixing and heat transfer. Figure 3 gives the bubble behaviour around a tube. There was a cycle including bubble passage, wake impact on tube and wake passage. The bubble wake was found to be important to the tube erosion.

References:

[1] Bouillard, J. X., Lyczkowski, R.W., Powder Technology, 68, 1991, 37-42.

[2] Lyczkowski, R.W., Bouillard, J. X., Progress in Energy and Combustion Science, 28, 2002, 543–602.

[3] Johansson, K., et al., Chemical Engineering Science, 59, 2004, 31-40.

[4] OpenFOAM User's guide, OpenCFD Ltd., UK, 2010.

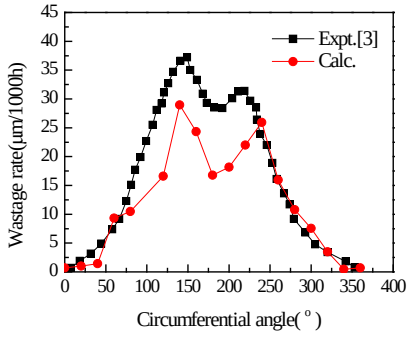

Fig. 1 Simulated wastage rates of the target tube compared with experimental data.

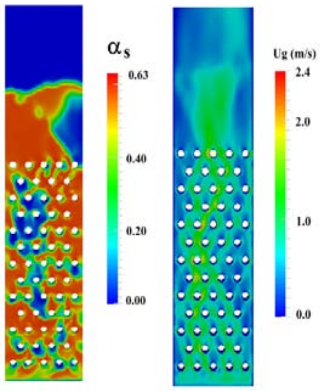

Fig. 2 Solid volume fraction and gas velocity at 4.5s for superficial gas velocity Ug = 0.4m/s.

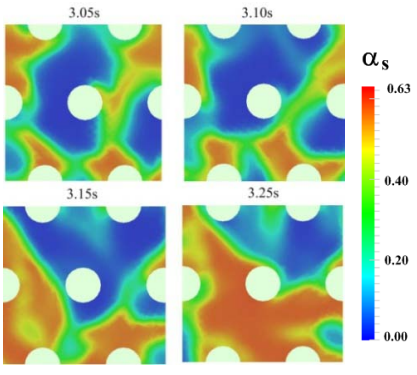

Fig. 3 Simulated bubble behaviours around the target tube at a series of time.

Thin film membrane for solid-state micro-batteries

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The ion-conducting polymer electrolyte in thin film format is important in the fabrication of light weight and shape-flexible solid state micro-batteries. Thin hybrid films based on block copolymer electrolyte, lithium salt and inorganic nanoparticles are investigated using optical microscopy, atomic force microscopy, scanning electron microscopy and grazing incidence small angle x-ray scattering. The structure of the hybrid films are examined as a function of Li/PEO ratio and nanoparticles content. Below a critical concentration cLi/PEO the crystallization of PEO is prohibited and nanostructured block copolymer films with Li incorporated in the PEO domains are obtained [1]. In a concentration regime above cLi/PEO aggregation of Li salt at the polymer film surface occurs due to limited capability of the PEO to accommodate the Li ions in the thin film geometry. The ionic conductivity of the hybrid nanocomposite films are measured using impedance spectroscopy. The effect of the hybrid electrolyte thin film composition/morphology on the ionic conductivity is demonstrated.

[1] E. Metwalli, M. Nie, V. Körstgens, J. Perlich, S.V. Roth, P. Müller-Buschbaum, Macromol. Chem. Phys. 212, 1742-1750 (2011).

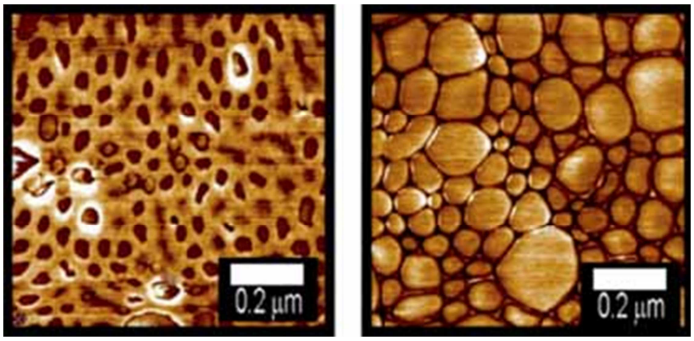

Fig. 1 AFM phase images indicate that the incorporation of lithium salt in block copolymer electrolyte thin films prohibits PEO chain folding and crystallization. Instead, a microphase separation process is dominant, and nano-sized cylinders of PS domains in a PEO matrix are formed. *(Left)* While, upon further increase of the lithium salt concentration (Li/PEO weight ratio > 0.015) aggregates of lithium salt on the surface are observed. (*Right*)

Beating the heat atomistically: Watching phonons cool down during O_2 dissociation on Pd(100)

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Energy conversion at interfaces is at the center of the rapidly growing field of basic energy science. One particular example is the conversion of chemical energy into heat which comes as an unavoidable by-product of all exothermic elementary reaction steps in heterogeneous catalysis. While engineers routinely deal with important consequences on a macroscopic scale based on well-known continuum theories and empirically determined effective parameters, an atomistic understanding is very limited at best.
Aiming at multiscale modeling, our novel QM/Me approach extends the power of embedding techniques to metallic systems. A huge atomistically described bath can thus be included in *ab-initio* molecular dynamics simulations of chemical reactions at catalyst surfaces. Applied to O_2 dissociation on Pd(100) as a representative showcase system, for which electron-hole pair excitations are unlikely to act as dominant primary energy dissipation channel [1], we quantify concomitant phonon excitations based on a newly developed projection scheme. Thanks to the phononic details implicitly incorporated in the bath, we obtain a high resolution for individual modes over the entire surface Brillouin zone. We can thus unravel the role of surface phonons as well as question the validity of the harmonic approximation for the solid during the dynamics - commonly employed in model Hamiltonians - from an unprecedented first-principles perspective. Finally, Fourier's law is revisited on an atomic scale.

Numerical Simulation of Cavitating Flows with Focus on Cavitation Erosion

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Motivation

The topics of cavitation and energy efficiency overlap in various fields. The most popular are surely hydropower (pumps and turbines) and combustion engines (injection systems). While in pumps and turbines the most efficient operating point often includes incipient cavitation, operating conditions in injection nozzles are typically chosen in a way that makes cavitation unavoidable.

Physical Background

The acceleration of a fluid leads to a drop in static pressure. If the pressure drops below the vapor pressure the fluid can rupture and form regions filled with vapor. This phenomenon is called cavitation. If generated vapor structures get advected into regimes of high ambient pressure the collapse-like recondensation leads to enormous instantaneous pressures and the formation of shockwaves in the liquid, potentially resulting in noise, vibration, or even erosion.

The resulting 2-phase flow includes challenging features such as local variation of density ($O(10^5)$), pressure ($<10^4$ Pa in 2-phase regime to $>10^8$ Pa in the center of a vapor-collapse), and speed of sound (<1m/s in 2-phase regime to >1000m/s in pure fluid). Furthermore, time scales of the underlying shear flow and propagating shockwaves typically differ in orders of magnitude.

Objective of the Contribution

We present our recent progress concerning the numerical simulation of 3-D unsteady cavitating flows with special emphasis on the prediction of cavitation erosion. We apply our flow simulation tool CATUM (Cavitation Technische Universität München) to simulate two different nozzle-target geometries (first shown in Fig. 1 and 2). Through a comparison with experimental results we demonstrate the ability of CATUM to identify erosion endangered material surfaces and provide information about erosion aggressiveness.

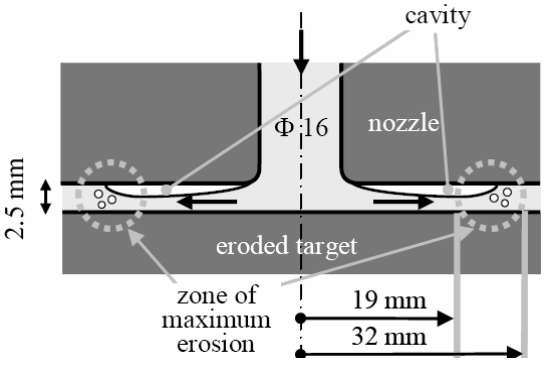

Figure 1 (up): Sketch of the axisymmetric experimental setup: a nozzle is directed onto a target body creating a radial divergent gap. At the exit of the nozzle the acceleration of the fluid along the radius leads to a transient cavitation pocket.

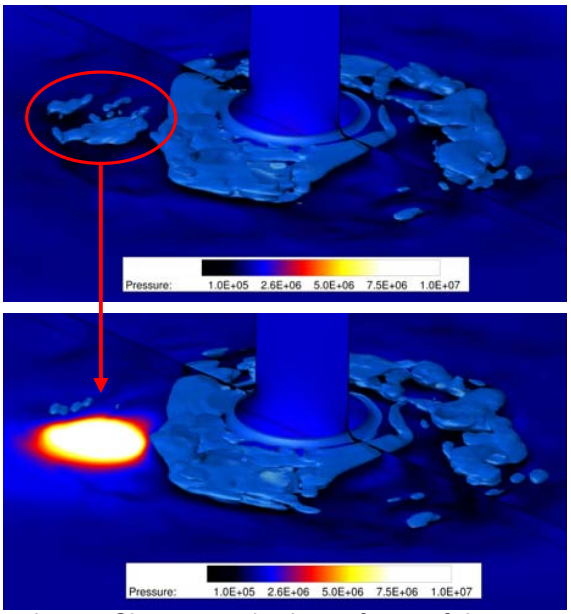

Figure 2 (right): Numerical simulation of the cavitation erosion experiment. Shown are the isosurfaces of the vapor volume fraction (0.1) and the static pressure on the lower wall of a radial divergent gap flow for two consecutive time instants ($\Delta t=28\cdot10^{-6}$ s). Top: Isolated vapor structure lust before collapse (red cycle). Bottom: Flow field after collapse with a collapse induced shockwave propagating through the liquid.

Biomass upgrading processes

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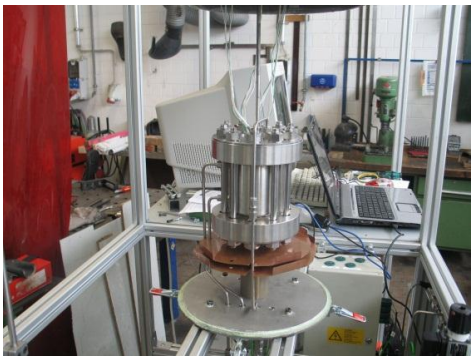
The actual idea of the substitution of fossil by biomass fuels is dealing with the questions of low energy density, heterogeneous quality and limited availability of this renewable energy. These disadvantages are complicating the utilization in industrial scale and causing lower efficiencies of the processes. To improve this, in the last couple of years different biomass upgrading technologies have been developed or taken up again. Especially for wet biomass, in reactors of high temperature or pressure the methods of Hydrothermal Carbonisation, Torrefaction or Hydrothermal Liquefaction can considerably increase the volumetric energy density. The results are upgraded fuels known as biocoal or biooil, which can be used in combustion or gasification processes. Further applications like the usage in coal or oil based products are feasible. In “Terra pretta” projects the improved coals enhance the water and mineral storage capacities of low quality soils.

The poster is going to estimating the quality of different biomasses and should give a brief introduction to these technologies and the possible fields of application. Furthermore some examples of applications are given and the energy efficiencies are compared.

A facility called HydEx-V is introduced, which is capable of studying these processes up to 200 bar and 500°C by recording the energy flows into and out of the system.



Fabrication of custom tailored titania nanostructures and hybrid thin films for application in photovoltaics

Martin A. Niedermeier[a], Monika Rawolle, Philipp Lellig, Volker Körstgens, Eva M. Herzig, Adeline Buffet, Stephan V. Roth, Jochen S. Gutmann, Thomas Fröschl, Nicola Hüsing, Peter Müller-Buschbaum[b]

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The search for alternative ways to accommodate the world's need for energy has been the subject of many researches in the last decades. Utilizing the sun as a virtual unlimited battery is a possible way for harvesting energy without harming the environment.
Amongst the numerous representatives, thin film solar cells are one potential candidate to cope with tomorrow's energy demands. One of them is the dye sensitized solar cell (DSSC), also known as Grätzel cell. Its distinctive feature is a nanoporous titania film, whose effective surface is increased by several orders of magnitude compared to a bulk film. This increase is directly transferred to the absorption of sunlight by the dye covering the titania surface 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.

In the presented investigation nanoporous titania films are tailored to the needs of DSSCs. For the preparation of our films we use a block copolymer as a structure directing agent and a liquid precursor to obtain crystalline titania film. By simple adjustments of the preparation conditions, various morphologies are accessible. Thus, along this route, complex hierarchical structures can be custom tailored [1].

A major drawback of the DSSC in terms of economic feasibility is the liquid electrolyte which is still the issue regarding significant sealing, and therefore, lifetime problems. One way to overcome that problem is to replace the liquid electrolyte with a solid hole conductor. These solid-state DSSCs, or also called hybrid cells if no dye is used, combine the advantages of the inorganic material, e.g. titania, with the strengths of organic materials, like being flexible, cheap and easy to manufacture.
We use a low-temperature process, in which the polymer and the semiconductor matrix are fabricated simultaneously. By optimization of the process parameters, suitable hybrid films are manufactured.

[1] M. Rawolle, M.A. Niedermeier, G. Kaune, J. Perlich, P. Lellig, M. Memesa, Y.-J. Cheng, J.S. Gutmann, P. Müller-Buschbaum, Chem. Soc. Rev. (2012), DOI: 10.1039/c2cs15321a.

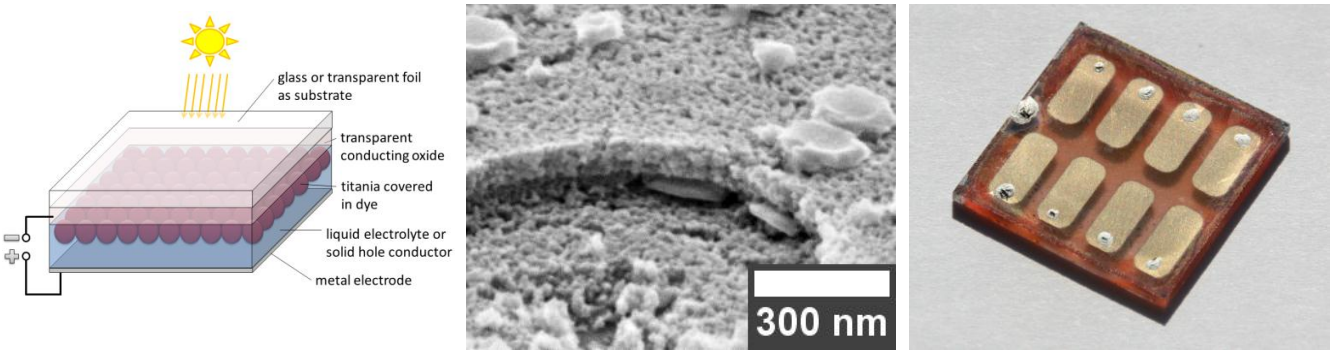

Fig. 1 (left to right): Sketch of titania based photovoltaic device, SEM close-up of layered titania nano-foam, and example of a titania-based solid-state DSSC.

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Structured Interfaces in Organic Photovoltaic Devices

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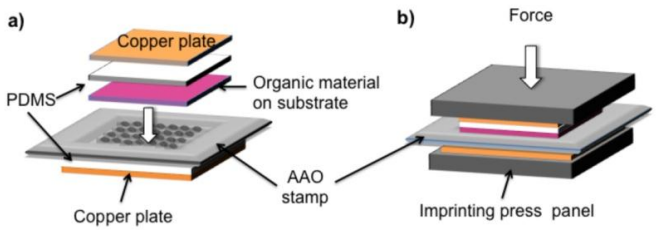
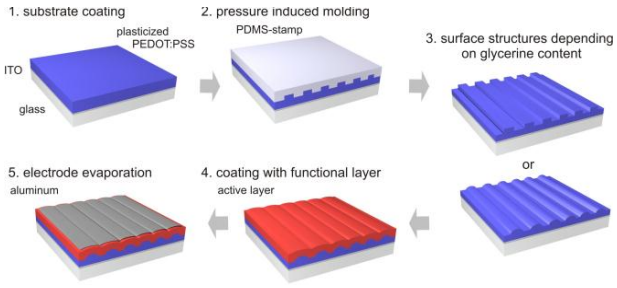
Precise control of the heterojunction morphology in thin films is one of the key issues for the improvement of organic photovoltaic (OPV) devices. Interdigitated interfaces of the organic material on the nanoscale provide ideal charge extraction pathways for separated charge carriers. Structured surfaces of the selective electrode on the lower microscale further allow for the enhancement of the optical absorption of the thin film components due to light trapping. Two different ways of artificial structuring are under investigation: Using anodized aluminum oxide (AAO) hard templates as stamps nanostructured organic layers can be realized on ITO support. Precise control of the anodization process facilitates the control of the template dimensions. As shown recently, a sufficient replica of the template structure can be transferred into the organic compound [1]. Experience in fabrication techniques including solution processing and vacuum sublimation techniques as well as different device geometries [2] enable it to study the device physics of these novel architectures in OPV devices. We investigate thermal and oxygen diffusion degradation processes of the imprinted layer. Furthermore, charge carrier dynamics in dependence on the illumination intensity are investigated for bilayer and nanostructured devices in comparison by intensity dependent photovoltage and photocurrent decay (PVD/PCD) measurements. Alternatively, a novel imprinting routine for polyethylenedioxy-thiophene:polystyrene-sulphonate (PEDOT:PSS) is studied as it is widely used as a selective intermediate electrode in OPVs blocking the electrons and collecting the holes. Thereby, master molds with nanoscale channels are used for the temperature and pressure assisted imprinting routine. The shape of the imprinted structures is easily tunable by the concentration of an additional plasticizer. Depending on the structure dimensions the device efficiency of OPVs can be increased this way [3]. This improvement is addressed to additional optical diffraction at the PEDOT:PSS gratings leading to increased optical absorption due to light trapping.

[1] Hesse, H.C., D. Lembke, L. Doessel, X. Feng, K, Müllen and L.Schmidt-Mende, Nanotechnology, 2011, 22, 055303
[2] Weickert, J. H. Sun, C. Palumbiny, H.C. Hesse and L. Schmidt-Mende, Solar Energy Materials and Solar Cells, 2010, 94, 2371
[3] Meier, R., C. Birkenstock, Claudia M. Palumbiny and P. Müller-Buschbaum, submitted



Imprinting process for structured donor-acceptor interfaces



Soft embossing imprint for PEDOT:PSS

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Silicon Based Electrolytes for Lithium Sulfur Silicon Batteries

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A new concept to increase the range of electric cars is the “Development of Lithium Sulfur/Silicon Batteries with High Specific Energy Density for the Automotive Application”. This new type of energy storage device combines a Li_2S cathode with a Si anode and will thereby offer a high specific energy density up to 450 Wh/kg on cell level. Besides the electrodes and other battery materials, new electrolytes are investigated as they have to fulfill certain properties.

This research concerns synthesis and characterization of electrolytes based on silicon containing cyclic carbonates. The systematic variation of different structural parts leads to a structure-property relationship with respect to electrochemical and thermal performance. Variation of a spacer between the carbonate unit and the silane unit, as well as different substituents at the silicon have so far been investigated. Therefore the conductivity of various compounds doped with different lithium ion conducting salts was investigated, as well as the electrochemical stability using cyclic voltammetry. In terms of thermal stability thermogravimetric analysis and differential scanning calorimetry are used to investigate the temperature range in which the battery can later on transfer lithium ions and operate.

Energy Management inside the own campus

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One challenge and - may be the important one of the future energy management - is the strategy to save energy. It has to be implemented everywhere in our residential and working environment especially at the own university campus.
Two main starting points could be identified to introduce to an energy saving strategy; implementation of a technical regulation facilitiy and the behaviour of the employees and students.

Steps of implementation

The Strategy of the Faculty Center of Life and Food Sciences Weihenstephan (WZW) started with the declaration of environmental guidelines in 2008.
An environmental and resource manager was appointed but only on part time work. A successful energy saving strategy has to be based on a data baseline of energy consumption - heat for the rooms and technical processes, electrical energy and water use.
So in 2010 the project “Ganzheitliches Energiekonzept für die Liegenschaften der Hochschulen in Weihenstephan - Providing a integrated energy concept for the properties of the university” (funded by Federal Ministry of Environment, BMU) the buildings of the TU München (WZW) and the Hochschule Weihenstephan-Triesdorf (HSWT) where checked concerning the energy and water consumption on a data basis from the year 2008.
In total there are 75 buildings with an area of more than 230.000m² and additional 12.000m² of greenhouse area. The whole campus of Weihenstephan, including buildings of other institutions has an energy uptake 72 Mio kWh, which is an emission of more than 27.000 t of CO_2. Fig. 2 shows additionally that electricity production emitted more CO_2 compared to district heat production; TUM-WZW takes off 59% of heat, 56% of electric power and 54% of the CO_2 emission. The benchmarking of the buildings compared the energy and water consumption to reference values, which are known for comparable buildings. The results showed large variations and gave hints to check some of them more intensively.
In a second step possible savings were checked for different technical investments but also the effect of changes in use by the employees was calculated. Overall investments in electrical techniques will have the best effects on CO_2 reduction (
Fig. 1). The change of heat production to a WZW-own energy plant was not competitive after a new contracting for district heating.
Technical investments can lead to a CO_2 emission reduction but need high capital. It is expected that employees can also reduce the energy consumption by own ideas and special continuous informations.

Further steps

The project results forced us to establish a core group for the campus Weihenstephan including also the Bavarian research centres. It is the ideas to implement an Energy management system which was part of the recommendations of the project report.
It was obvious that all investments and also informations and instructions for the employee need a detailed registration and documentation of energy consumption. In the moment it is not realized, and it seems that investments are far away.
What could be down on a lower level of investment?
This year the Immobilien Management will invest in LED light for the ways at the campus Weihenstephan and in one lecture hall the filament lamps will be changed to LED as well.
In a TU subunit, the Z I E L - Research Center for Nutrition and Food Sciences, a group of very interested people of the staff develops strategies for lower energy consumption f.ex. adapted periods a heating and room temperatures, roles for air condition and gives information to the whole staff by newsletters.
Another idea is to develop new electronically register tools for old analogue register units to change them to way of smart metering. This should be a challenge for students and could be cheaper compared to new ones.
At least, the campus with its facilities and infrastructure is great challenge for everyone who is interested in energy management and energy saving. Students and scientist are invited do research and applying their technical expertise on their own campus.

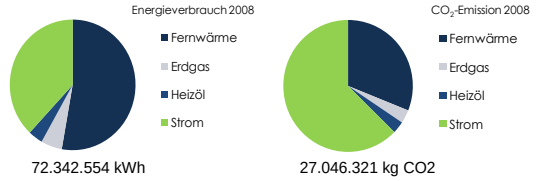

Fig. 2 Total and percentual energy consumption as heat, gas, oil (direkt), electric power and CO_2 emission of each source at the campus Weihenstephan

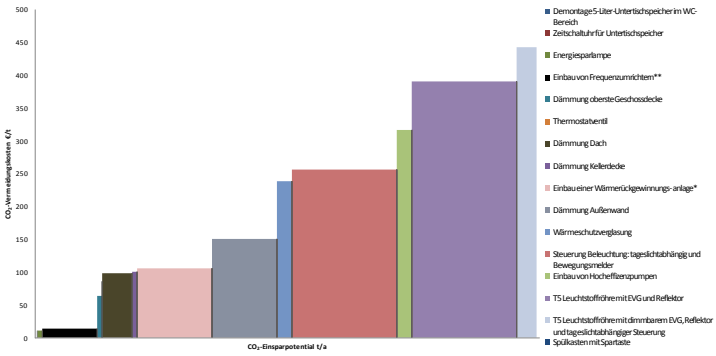

Fig. 1: Potential of CO2-emission reduction related to costs

Study of Hydrogen Oxidation and Evolution Reaction Kinetics in Alkaline Electrolytes using Rotating Disc Electrode Voltammetry

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Fuel cells have been recognized as an efficient technology for the conversion of chemical energy into electricity. Owing to their high power densities, certain kinds of low-temperature fuel cells comply with the requirements for automotive propulsion systems, where the use of Proton Exchange Membrane Fuel Cells (PEMFCs) with an acidic polymer electrolyte (typically a Nafion® membrane) is generally envisaged[1].

Due to the low operative temperatures, the electrochemical reactions taking place inside the fuel cell demand efficient catalysts in order to achieve the required power output. In PEMFCs this catalyst typically consists of platinum nanoparticles supported on carbon black, and is responsible for ≈ 50 % of the stack's cost[2]. While the hydrogen oxidation reaction (HOR) on Pt is fast in this acidic medium, the oxygen reduction reaction (ORR) shows very slow kinetics and thus 5 – 10-times higher platinum loadings are required at the PEMFC's cathode[3]. In contrast to the acidic system, fuel cells with alkaline electrolytes (Alkaline Fuel Cells, AFCs) allow the application of non-noble metal-based cathode catalysts with ORR activities comparable to platinum[4]. However, the essential drawback in this case is the rather high overpotential for the HOR on Pt at the anode side[2], rendering the development of efficient catalysts for this reaction a fundamental challenge in the evolution of AFCs.

With this motivation, our research focuses on the effects of electrolyte alkalinity and the nature of the catalyst on HOR/HER(hydrogen evolution reaction) kinetics. For this purpose we have performed rotating disc electrode (RDE) voltammetry on polycrystalline platinum[Pt(pc)] and palladium [Pd(pc)] in aqueous solutions of 0.1 and 1.0 M KOH, at temperatures between 0 °C and 80 °C. As an example of our results, Figure 1 shows a comparison of the HOR/HER current densities on Pt(pc) in different concentrations of KOH at 20 °C, and illustrates the strong decrease of the limiting current as a result of the higher alkalinity.

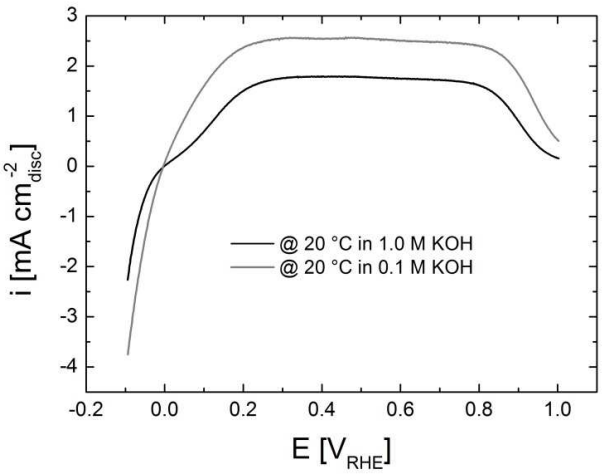

Figure 1. HOR/HER current densities recorded on a Pt(pc) RDE at 1600 rpm and a sweep rate of 10 mV s^{-1} in H_2-saturated aqueous solutions of KOH.

In summary, this contribution will show the influence of these parameters on the HOR/HER kinetics in alkaline solutions.

[1] S. Lu, J. Pan, A. Huang, L. Zhuang, and J. Lu, *PNAS*, **105**, 20611 (2008).
[2] B. D. James, J. A. Kalinoski and K. N. Baum, http://www1.eere.energy.gov/hydrogenandfuelcells/pdfs/dti_80kwW_fc_system_cost_analysis_report_2010.pdf, 2010.
[3] W. Sheng, H. A. Gasteiger, and Y. Shao-Horn, *J. Electrochem.Soc.*, **157**(11), B1529-B1536 (2010).
[4] M. Piana, S. Catanorchi, and H. A. Gasteiger, *ECS Trans.*, **16**(2), 2045 (2008).

Designing Business Models and Prototypes for Future Energy Systems: A Micro Grid Office Solution

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Information and communication technologies will be needed in future energy systems in order to integrate a large share of renewable energies and cope with the problem of fluctuating electricity generation. Even though experts mainly agree on that, it is unclear how future technical components of such systems may look like and how profitable business models could be designed. To tackle this problem and accelerate the adoption of smart energy technologies and the transformation of our energy system, we work on future business models and prototypes that create value for all involved stakeholders.

In this work, we present a business idea for a micro grid office building solution. The two parts, a business plan and a prototype have been developed using an innovative business modeling approach. The business development methodology consists of various interdisciplinary teams, weekly lectures and coaching sessions and a project for each team. Each team consists of four or five students with different backgrounds. The teams work on their specific product development task, which was prepared and conceptualized by research assistants and industry partners. During this project students get insights into important product development areas as for example: techniques for user need studies, market and competitor analysis, business modeling, mockup demonstration, and prototyping. At the end of the development project, students are able to apply the product development process on a specific technology project.
One of these teams developed an innovative solution for a micro grid in an office building. The team was supported by experts from academia as well as industry partners and got further inputs by talks and excursions specifically on the topic of smart energy systems.

The poster shows the general concept of this developed smart energy system solution called Griddle.
Griddle is an application-based service that helps and incentivizes office employees to save energy and to adjust their consumption behavior to the current microgrid status. Thereby it helps to overcome major challenges that microgrids face in a smart commercial building environment: Aligning the consumption to the volatile energy production and being independent from the main grid – both resulting in cost inefficiencies within microgrids.
Griddle's unique problem-solving approach is user involvement instead of automation. This is realized by a personalized application that runs on smartphones and a webpage that is displayed on TV screens. On one side the application receives push notifications concerning suggestions for grid conscious consumption and allows gamification by the use of competition. On the other side the screen ambiently arouses awareness and thereby indirectly notifies the user of the current microgrid status. This combination of different devices leverages microgrids and cuts companies' energy consumption costs by up to 20%.

References:

[1] BDI (2008): Internet der Energie - IKT für Energiemärkte der Zukunft.
[2] Darby, S. (2006): The effectiveness of feedback on energy consumption, Environmental Change Institute, University of Oxford.
[3] Petkov, P. et al. (2011): Engaging energy saving through motivation-specific social comparison, Annual conference on human factors in computing systems (CHI).

Research Project HotVeGas II

F. Botteghi, C. Erbel, M. Losurdo, M. Nakonz[a], R. Rück[b], H.Spliethoff[c]

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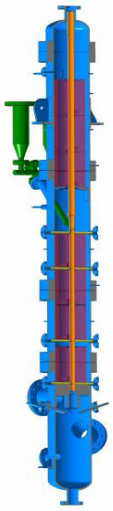
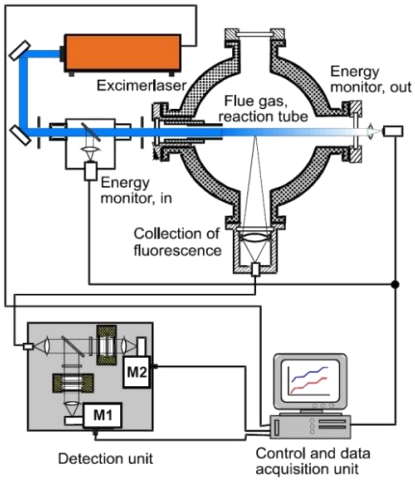
IGCC power plants, based on coal gasification, have the capabilities to compensate the inconsistent production of power in a future power generation mixture. They can be designed for high flexibility with a base load designed gasifier (8000h/a at 100%) and a combined cycle designed to specific requirements. When the gas turbine is not required, the synthesis gas can be stored for later or other use as chemical energy carrier. Therefore the IGCC power plant is very flexible in power generation and gas production. High efficiency and low emissions are additional benefits of the IGCC plant compared to conventional coal fired power plants. Gasifiers can handle a wide range of fuels, coal, biomass and waste, and can contribute therefore to a secure and cost efficient power generation.
To build power plants with highest efficiencies and usability it is necessary to gain more knowledge about the basic processes as well as the detailed reactions of the gasification and the behavior of trace elements, which are critical for corrosion effects.
The HotVeGas Project is dealing with all aspects from simulation of reactions and gas flows over experiments in multiple sized reactors for all steps of pyrolysis, gasification and trace element behavior in the cooling gas flow. Different measurement technologies are used and developed for very special investigations. Available reactors are a pressurized flow reactor (PiTer), an atmospheric flow reactor (BabiTer), pressurized thermo gravimetric reactors (PTGA), a pressurized gas cooling line with external alkali evaporator (AKS) and others. Some of the reactors can reach temperature and pressure conditions that have been rarely investigated worldwide but are very interesting with regard to future IGCC plants. The sizes reach from 7 m of the PiTer to only mm in the PTGA. This offers the possibility to investigate a wide range of aspects and also validate scale effects and simulations.



Gasifier „PiTer“

CFD Simulation



ELIF alkali measurement

Hybrid films based on zinc oxide network structures for applications in organic photovoltaics

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The role played by the inorganic nanostructures in the field of energy conversion has dramatically intensified by the contribution from the hybrid photovoltaic devices such as light emitting diodes and solar cells. Solar energy serves as the most abundant source for green electricity which has triggered the fabrication of photovoltaic devices in the past two decades for the generation of electric power to answer the increasing demand. Organic as well as hybrid solar cells have been studied which promise reduced fabrication costs, simple processing and employment of flexible substrates. However, hybrid solar cells are of greater interest as they provide the benefits associated with both the organic and the inorganic material.

Hybrid dye sensitized solar cells conventionally prepared using titania as the inorganic material have reached power conversion efficiencies up to 11 % [1]. As an alternative to titania, zinc oxide (ZnO) is used in the present study. This is possible due to very similar optical and electronic properties of ZnO to titania and in addition, its high mobility in the bulk [2]. A power conversion efficiency of 4.7 % has been reported for a dye-sensitized hybrid solar cell incorporated with spray-deposited ZnO nanoparticles [3].

Tailoring the ZnO morphology plays an important role in enhancing the effective surface area and interfacial interaction between the electron-accepting ZnO and an organic hole-conducting polymer. Hence, designing a suitable morphology of ZnO has been the main focus of this study. ZnO nanostructures are synthesized on silicon substrates forming different nanostructured morphologies consisting of foam-like structures, worm-like aggregates, circular vesicles and spherical granules. The synthesis is using a sol-gel mechanism coupled with amphiphilic diblock copolymers such as polystyrene-*block*-polyethyleneoxide, P(S-*b*-EO) and polystyrene-*block*-4-vinylpyridine, P(S-*b*-4VP) acting as structure directing agents. N,N-dimethylformamide is used as the good solvent and water as the selective solvent for both the diblocks. The ZnO precursor, Zinc acetate dihydrate (ZAD) is incorporated in the hydrophilic block. The different morphologies are obtained by adjusting the weight fractions of the solvents and ZAD. Thin film samples with ZnO nanostructures are prepared via spin coating and solution casting followed by a calcination step. A ternary phase diagram is plotted based on the various morphologies obtained showing their respective compositional boundaries. The surface morphologies of the ZnO nanostructures are studied with scanning electron microscopy (SEM). The inner structures of the samples are probed using grazing incidence small angle X-ray scattering (GISAXS). X-ray diffraction (XRD) measurements confirm the crystallization of the ZnO to the wurtzite phase upon calcination.

[1] Gao et al., *Chem. Commun.*, pp. 2635-2637 (2008)

[2] Bouclé et al., *J. Phys. Chem. C*, vol. 114(8), pp. 3664-3674 (2010)

[3] Rao et al., *Nanotechnology*, vol. 19, pp. 445712 (2008)

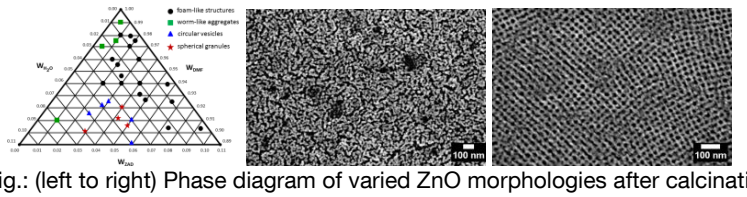

Fig.: (left to right) Phase diagram of varied ZnO morphologies after calcination, example of ZnO nano-morphology templated using P(S-*b*-EO) and P(S-*b*-4VP).

Degradation and aging in polymer solar cells

Christoph Schaffer[a], Matthias Ruderer, Shuai Guo, Peter Müller-Buschbaum[b]

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Polymer solar cells (PSCs) using thin polymer films to convert light to electric energy are successively gaining interest as a climate-neutral energy source. The comparatively moderate power conversion efficiency of yet little over 10%, is compensated by potential low production costs and the extensive possibilities of application: Thanks to mechanical flexibility and a variety of colors and shapes available, PSCs will be suitable to be placed broadly on claddings and windows, posing both functional and architectural elements. A major challenge restraining the commercial launch of PSCs lies in the yet short lifetimes of a few years at maximum. It is well known that illumination in an oxygenic atmosphere can lead to photo-bleaching of the active polymer layer and to oxidation of the metal contacts and polymers, thus causing a decay of performance which can though be overcome by use of an adequate encapsulation. However, the impact of environmental stresses on the structural and interfacial characteristics of the polymer layer on a nano- and micrometer scale is not sufficiently studied.

Our main objective is consequently to emulate and evaluate the environmental impact on the morphological and structural properties in a model system (PTB7:PC71BM and P3HT:PCBM respectively) due to oxygen, humidity, temperature and long-term illumination in distinct spectral ranges and to correlate the findings to the optical and electric characteristics of the photovoltaic devices. Therefore, long-term illumination of PSCs will be performed under well defined atmospheric conditions. Insight into the structural properties of thin polymer films between a sub-nanometer and a micrometer scale is thereby gained by advanced scattering methods. Direct imaging techniques such as scanning probe and optical microscopy provide complementary knowledge of the thin film morphology.

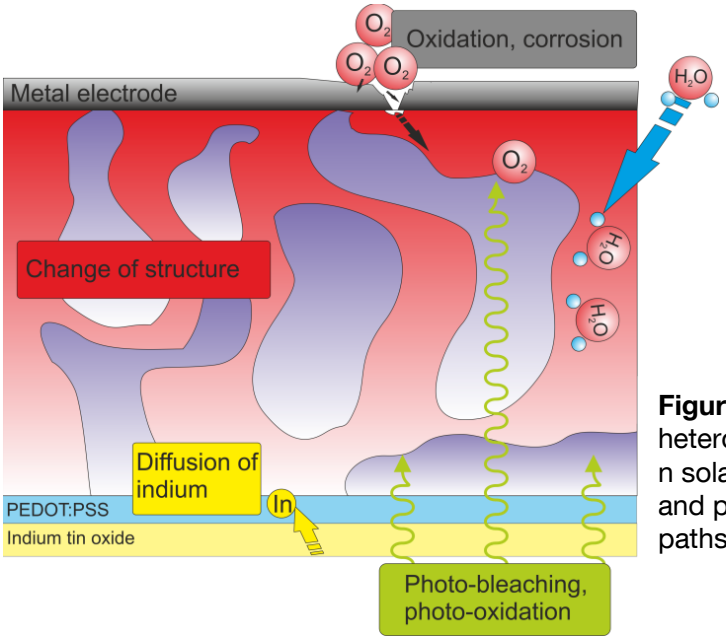

Figure: Bulk-heterojunction solar cell and possible paths of

Tuning Photocatalytic Hydrogen Evolution by means of Size-Selected Pt Clusters on CdS Nanorod Films

Florian F. Schweinberger[1]*, Maximilian J. Berr[2], Markus Döblinger[3], Martin Tschurl[1], Frank Jäckel[2], Jochen Feldmann[2], Ueli Heiz[1]

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Solar hydrogen production has recently gained renewed interest in photocatalytic hybrid nano particle systems, utilizing colloidal semiconductor nanoparticles as sunlight absorber with additional nobel metal nanoparticles as hydrogen catalyst [1-3].

In spite of its high cost and rareness Pt nanoparticles still remain the most frequently used catalysts for photocatalytic hybrid nano particle systems due to its simple photochemical deposition methods and high catalytic activity [1-2].

Recently it has been demonstrated that the total Pt amount can be reduced significantly employing sub-nanometer Pt cluster instead of nanoparticles without decreasing the overall photocatalytic quantum efficiency[1].

By soft-landing deposition of size-selected Pt clusters under UHV conditions [4], we present a novel and alternative decoration method for colloidally synthe-sized CdS-nano rods. Therefore a CdS-nanorod film was spin-coated onto an ITO substrate and decorated with Pt clusters of defined size (size-control down to a single atomic mass) and precisely controlled coverage in an UHV setup using a laser-ablation cluster source.

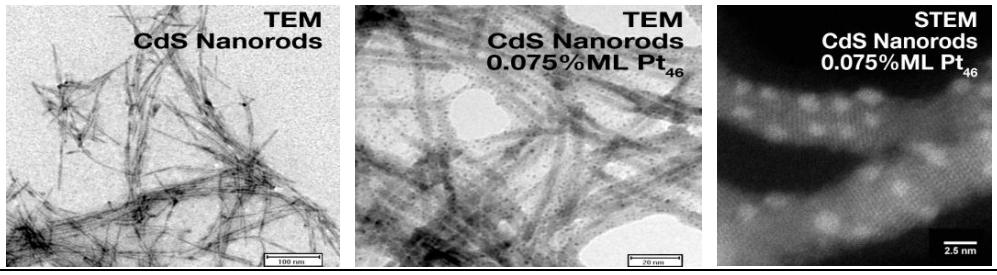
Subsequently, quantum efficiencies were measured in an aqueous solution of triethanolamine (TEA) as a hole scavenger under UV illumination in dependence of average number of clusters per nanorod and cluster size.

[1] M.J. Berr, A. Vaneski, A.S. Susha, J. Rodríguez-Fernández, M. Döblinger, F. Jäckel, A.J. Rogach & J. Feldmann. *Appl. Phys. Lett. 97*, 093108 (2010).

[2] L. Amirav, A.P. Alivisatos. *J. Phys. Chem. Lett.* 1, 1051 (2010).

[3] Y. Shemesh, J.E. Macdonald, G. Menagen, U. Banin. *Angew. Chem. Int. Ed.* 50, 1185 (2011).

[4] S. Kunz, K. Hartl, M. Nesselberger, F.F. Schweinberger, G. Kwon, M. Hanzlik, K.J.J. Mayrhofer, U. Heiz & M. Arenz. *PCCP* 12, 10288 (2010).



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Analysis of the Challenges Posed on the Power Grid by Renewable Energies and Electric Vehicles and Potential Solutions

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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. electric vehicles. The 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 are expected to gain popularity and market share over the next few years. 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 Institute of Power Transmission Systems is investigating concepts on integrating electric 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. 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 electric 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 Institute of Power Transmissions Systems is investigating different scenarios for the optimal use 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.

In order to transmit the power generated by off-shore wind parks to the load centers, new transmission lines are necessary. The Institute of Power Transmission Systems is investigating how gas-insulated transmission lines (GIL) can help to solve this problem. GILs combine numerous advantages of cables and overhead lines e.g. they are buried underground and thus have less problems with authorization, a low capacitance and a high thermal transmission capacity.

The integration of renewable energy generation systems leads to a replacement of rotating masses with power electronics. This might lead to stability problems. In order to evaluate the influence of power electronic converters on the system stability, the German transmission system has to be modeled and analyzed.

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Energy Systems Modelling – A Grid Perspective

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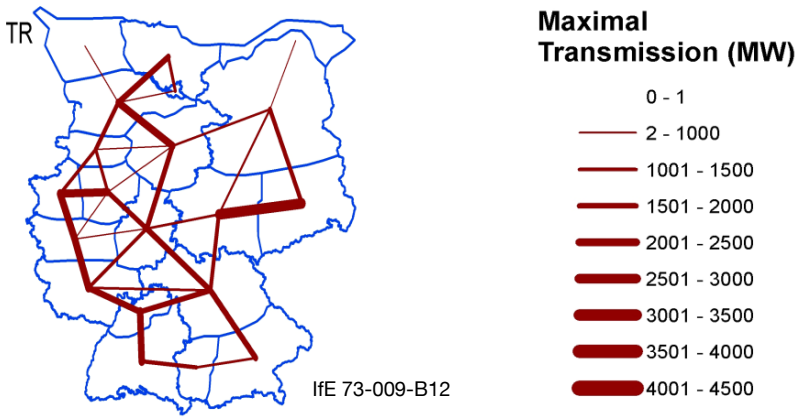
Sustainable energy systems for the future require rethinking established ways to meet electricity demand.
When attempting to formulate requirements for a German energy system in 2050 in the light of climate change and recent political decisions, an increased feed-in of renewable electricity generation must be considered.
This electricity generation is typically highly fluctuating and can only partially be predicted, posing new challenges to the system in order to match electricity generation and demand.
Energy system modelling can contribute at this point to defining optimal paths to build up an infrastructure that is ready to handle these challenges.

Within the scientific community, the simple unit commitment problem has already received much attention, also in the context of power plant portfolio expansion planning.
Grid and storage aspects, on the other hand, have till now not received as deep an investigation.
One reason for this is that these aspects lead to highly interconnected models in space and time respectively, which makes them difficult to solve with conventional methods.

Our poster will give a brief overview of the most widespread models used for electricity network representation in the context of holistic electricity generation, transportation and storage modelling on a European level. These models are:
the copper plate model, which neglects network constraints altogether, the transport model (a simple network flow model), the DC model (which enhances the transport model with additional constraints regarding Kirchhoff's laws) and exact physical AC-calculations.

We compare line load as well as the feasibility with different models to obtain results regarding the effects of simplifications made by the different models. On this basis, we outline extensions to some models that increase the degree of detail without compromising too much on computational performance, thus maintaining the applicability in the context of modelling entire energy systems.

We further give examples, how the inclusion of network constraints of different complexity influences the results of our combined infrastructure expansion and unit dispatch model, which also covers the usage of storage facilities.



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Binary compounds in the system Li-Si as novel anode materials for next generation Li-Ion batteries

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Renewable energy sources and new, highly efficient ways of energy storage are the challenges for the future. With the advent of electromobility, the research on Li-Ion batteries as energy storage units gained the upmost relevance. High capacities and long lifetimes are necessary for batteries to win the challenge. In this respect, recent focus has been turned on silicon as alternative anode material to the commercially used graphite. While graphite offers a specific capacity of 372 mAh/g, silicon arrives, in the Li-richest phase, to a theoretical capacity of 4008 mAh/g[1]. The outstanding capacity and its abundance on the earth's crust make silicon one of the most promising candidates as anode material for next generation Li-Ion batteries. Therefore the study of Si-containing materials is of vital importance for the development of high-performance Li-Ion batteries.

In this project we focus on the synthesis and characterization of binary compounds in the system Li-Si. The Li-Si phase diagram proposes a wide range of binary compounds[2], all of them already known. Binary Li silicides are here prepared via mechanical milling and annealing at 500 °C of the pure elements[3]. Structural characterization of the prepared phases is carried out via X-Ray Powder and Single-Crystal Diffraction (XRD), Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Spectroscopy (EDX), while electrochemical measurements, such as impedance spectroscopy and cycle-voltammetry, are performed in order to understand the behavior of the synthesized phases as anode materials.

[1] Y. Kubota, M. C. S. Escaño, H. Nakanishi, H. Kasai *J. Appl. Phys.* **102** (2007), 053704
[2] H. Okamoto *J. Phase Equilib. Diff.* **30** (2009), 118
[3] B. Key, R. Bhattacharyya, M. Morcrette, V. Seznéc, J. M. Tarascon, C. P. Grey *J. Am. Chem. Soc.* **131 (26)** (2009), 9239

Modified surface of CNT electrodes for flexible all polymer solar cells

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Recently, organic solar cells attract great attention due to the unique features, such as light weight, easy processability, potential low costs and flexibility. Presently, indium tin oxide (ITO) electrodes are the typically used electrodes in organic solar cells. Although these ITO electrodes have high transmission and high conductivity, their mechanical rigidity limits an application in flexible and large area solar cells. Moreover, the worldwide known amount of indium is extremely limited and will make a mass production cost-intensive. So a replacement of ITO electrodes is of interest. Among the most promising alternatives to ITO electrodes are carbon nanotube (CNT) films due to their higher flexibility, similar transmission and lower costs as compared to ITO electrodes. However, the disadvantages of CNT films, such as high surface roughness and low surface energy, still limit its application as electrodes in solar cells. Therefore, modifications of CNT electrodes are needed to improve the performance of the solar cells.

The surface morphology of CNT/PET electrodes is crucial for solar cell fabrication. So we first investigated the surface morphology of CNT/PET film with atomic force microscopy (AFM). As shown in Fig.1 a, the CNT are cross linked and bundled together, which contributes to the high conductivity for electrodes. However, it is also found that the surface roughness of CNT film is around 13 nm. Considering such high roughness, some CNTs could penetrate the active layer placed on top of the CNT film, which would result in a short cut of the solar cells. To address this problem, the PEDOT:PSS layer is coated on top of the CNT layer. The contact between the PEDOT:PSS and the CNT layers is critical for the solar cell performance. The better contact introduces lower parallel resistance, which gives rise to high short circuit current and high efficiency. Usually, O_2 plasma is selected to improve the surface energy of electrodes, which contributes to the good contact between PEDOT:PSS layer and electrodes. But for CNT film, the O_2 plasma degenerates the CNTs, which makes the CNT electrodes insulating. Therefore methanol is added to the PEDOT:PSS solution to replace the O_2 plasma treatment.

The surface morphology of PEDOT:PSS layer with different amount of methanol is investigated with AFM, which is shown in Fig.1. It is found that the PEDOT:PSS layers follow the surface morphology of the underlying CNT substrate and with increasing methanol content it is becoming more pronounced again which is evidence for the better wetting of the CNT film. The sheet resistance of all the films is also probed. It shows that adding methanol increases the sheet resistance, and the higher volume of methanol induces larger deviations, indicating that the film becomes less homogeneous.

In summary, adding methanol in PEDOT:PSS improves the wetting of PEDOT:PSS on CNT substrates, but a too high amount of methanol causes heterogeneities in the PEDOT:PSS films. Therefore, volume fraction of 33% methanol is the optimum condition in our investigation.

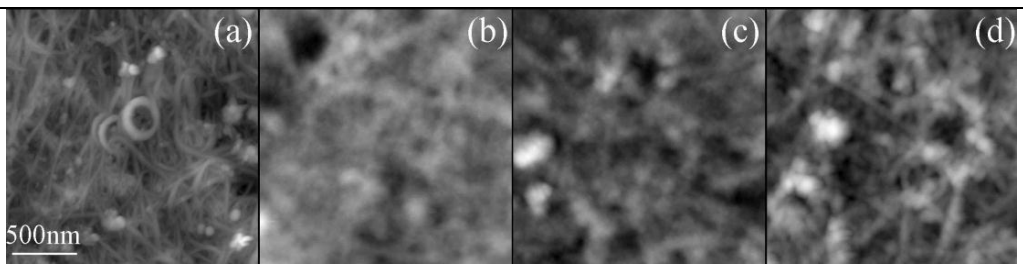

Fig. 1 AFM images of a) CNT film, b) pure PEDOT:PSS film, c) PEDOT:PSS film with 33% volume fraction methanol and d) PEDOT:PSS film with 75% volume fraction methanol)

Research for the Mass Production of Lithium-ion cells

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The success of the German “Energiewende” requires a number of measures in terms of power systems, energy storage and energy distribution. The extensive integration of renewable energy sources implies an increasing need of stationary energy storages in order to improve network stability, power quality and reliability of supply. Next to a multitude of existing and to be developed solutions, like flywheels, ultracapacitors, redox-flow-batteries and pumped storages, stationary batteries based on lithium-ion technology are an auspicious option especially for low and medium power applications. Although lithium-ion systems show significant capability and flexibility considering energy storage and power requirements, production costs of lithium-ion-batteries currently hinder their wide application. In order to reduce battery costs, new methods for the mass production of lithium-ion cells have to be developed. Therefore the Institute of Machine Tools and Industrial Management (iwb) of the Technische Universität München (TUM) has built up a research center for the production of lithium-ion cells, funded by the Federal Ministry of Education and Research (BMBF). Within the process chain for the production of lithium-ion cells anode, cathode and separator coils are assembled to cell stacks. 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 yield of the production system. 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. A trade-off between process speed by using continuous materials and the gentle handling of single sheets is the z-folding of the separator combined with single sheet electrodes. Due to the increased stacking speed and the optimized separator handling, this 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 cutting of the electrodes, providing a more flexible process which is free of tool wear and which shows a reduced burr. In order to detect particles that can occur within the laser cutting process a detection system for particles in the dimension of 20 microns is required. At the iwb the processes cell stacking by z-folding and laser cutting have been realized in two automated production modules including an optical system for the quality assurance of the electrode surfaces. In current research activities the implementation and investigation of the remaining steps of lithium-ion cell production and advanced methods for quality inspection, like thermo graphic systems, are addressed.



Figures: TUM Heddergott

Electrode optimization and behavior of LTO/LFP electrodes for applications in lithium ion batteries

Rebecca Zeh[a], Frank Kindermann[b], Ralph Karl[c], Hubert A. Gasteiger[d], Andreas Jossen[e]

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In order to reduce the consumption of fossil energies and to replace nuclear power plants, an appropriate storage system to store energy, from renewable sources like the wind and the sun, has to be developed. A battery system with a high cyclability, stable capacity and unhazardous substances is a suitable candidate. In 2010, Guerfi et al.[1] demonstrated that a battery system consisting of lithium titanate (Li4Ti5O12; LTO) and lithium iron phosphate (LiFePO4; LFP) shows a stable and constant discharge capacity for more than 20,000 deep cycles. Due to these results, the battery system LTO/LFP is a possible option for long term storage.

This project is a cooperation of the Institute of Technical Electrochemistry (TU München, Prof. Dr. Hubert A. Gasteiger) and the Institute of Electrical Energy Storage (TU München, Prof. Dr.-Ing. Andreas Jossen).

The goal of this work is to investigate the detailed degradation mechanisms of the LTO/LFP system and to get a better understanding of the processes inside the electrode. Therefore, we focus on the impact of electrode composition and temperature on the cycle life.

The individual cell design allows the measurement of the electrode combination with a reference electrode and the adjustment of a defined compressive force on the electrodes. We compared half-cell measurements of LTO and LFP electrodes versus a lithium counter electrode, with both thin and thick electrodes. Using electrochemical impedance spectroscopy and galvanostatic cycling procedures, we can show differences in the charge transfer resistance and the capacity for thin and thick electrodes. After a temperature treatment we can see changes in both, resistance and capacity.

[1] Guerfi et al. Journal of Power Sources 159 (2010) 845-852
[2] Christensen et al. Journal of the Electrochemical Society 153 (2006) A560-A56

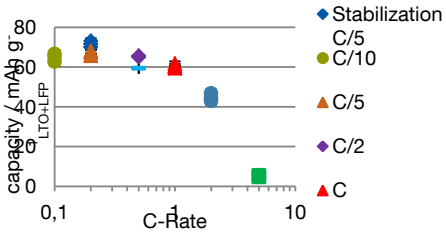

Figure 1: Discharge capacities of a LTO/LFP full-cell at different C-Rates at room temperature

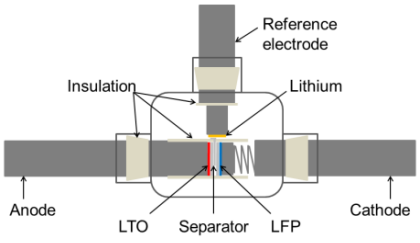

Figure 2: Schematic cell design of a LTO/LFP full-cell with the reference electrode. The current collector on the cathode side is featured with a spring, to set the pressure of the electrodes

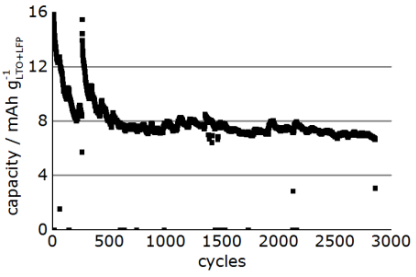

Figure 3: Constant capacity of LTO/LFP full-cell over 3,000 deep cycles with a charge/discharge rate of 1C

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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