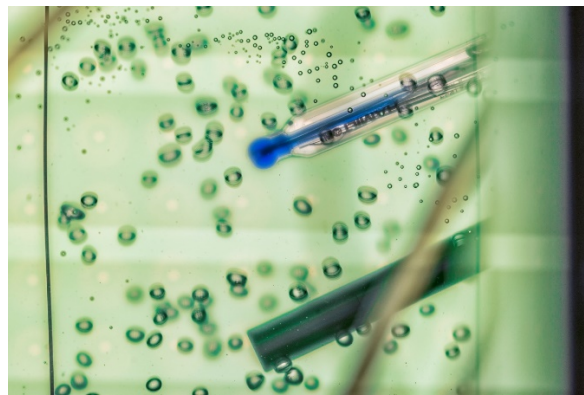


# Book of Abstracts



## UFZ EnergyDays 2019 “Sustainable Energy Carriers and Energy Storage/ Management”

October 8-9, 2019, KUBUS Leipzig

<https://www.ufz.de/index.php?en=101392&nopagecache>

## Introduction

The Helmholtz Centre for Environmental Research – UFZ welcomes you to the EnergyDays 2019 in Leipzig, Germany. The event aims to bring together UFZ colleagues in the field of energy-related research and to share and discuss experiences, research results, and directions covering all aspects of the eco-efficient production and storage of materials and energy carriers. This also includes exchange on future topics and collaboration opportunities in the frame of POF IV, where different energy-related research lines are distributed among different „Topics“ of the research program “Changing Earth – Sustaining our Future”.

The UFZ EnergyDays 2019 are organised by the Integrated Project (IP) Sustainable Biotechnology and Bioeconomy in cooperation with the IP Energy Land Use and the IP From Models to Prediction.

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# UFZ EnergyDays 2019: Sustainable Energy Carriers and Energy Storage/Management

8<sup>th</sup> and 9<sup>th</sup> of October 2019, KUBUS Leipzig

## Programme

Tuesday, 8 October 2019			
12:00	Registration		Foyer
13:00	Welcome and Introduction: Bruno Bühler, UFZ		Hall 1A
13:30	<b>Keynotes:</b> <ul style="list-style-type: none"> <li>Andreas Schmid, UFZ, <i>Engineering photosynthesis for decentralized hydrogen production from water- Status and perspectives</i></li> <li>Daniela Thrän, UFZ, <i>Energy and Bioeconomy</i></li> </ul>		Hall 1A
14:30	Coffee break		Foyer
15:00	<b>Session A1</b>	<b>Hall 1B</b>	<b>Session B1</b>
	<b>Workshop Session: Climate change and its impact on renewable energy sources</b>  <b>Chair: Katja Bunzel</b>  Renewable energy plays an important role in reducing greenhouse gas emissions and to mitigate climate change. However, the different renewable energy sources are also affected by climate change itself, via long-term changes in climate parameters, variability and extreme weather events. Mitigation and adaptation efforts might be hindered by that. Therefore, within this session, we want to discuss how we already incorporate these issues in our research and to identify open research questions.		<b>Storage (and waste): Biogeochemistry of energy underground storage</b>  <b>Chair: Carsten Vogt</b> <ul style="list-style-type: none"> <li>Olaf Kolditz, ENVINF, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Overview of iCross</i></li> <li>Laura Schwab, ISOBIO, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Biogeochemistry of hydrogen storage in salt caverns</i></li> <li>Michaela Löffler, ISOBIO, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Tracking hydrogenase activity with hydrogen stable isotope tools</i></li> <li>Nina-Sophie Keller, ISOBIO, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Monitoring of the fate of methane injected into a pristine near-surface aquifer using stable carbon isotope analyses</i></li> <li>Mohammad Sufian Bin-Hudari, ISOBIO, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Biogeochemical effects of temperature changes on microbial communities and groundwater contaminations</i></li> </ul>

16:30	<b>Coffee break</b>		Foyer
17:00	<b>Session A2</b>	<b>Hall 1A</b>	<b>Session B2</b>
	<p><b>STROMER</b></p> <p><b>Chair: Jens Krömer</b></p> <ul style="list-style-type: none"> <li>Jieying Zhou, TUCHEM, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Electrosorption of polar organic micropollutants on activated carbon-based materials</i></li> <li>Anh Vu Nguyen, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Getting electrons in and out of cells: sugar catabolism of Pseudomonas putida KT2440 in bioelectrochemical reactor</i></li> <li>Francesco Scarabotti, UMB, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>A closer look to the extracellular electron transfer in the model system Geobacter sulfurreducens</i></li> <li>Johannes Nelles, UBZ, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Scaling of electro(bio)reactors</i></li> </ul>		<p><b>Modelling and numerical analysis of coupled multiphysics processes of geological thermal energy storage</b></p> <p><b>Chair: Haibing Shao, Uwe-Jens Görke</b></p> <ul style="list-style-type: none"> <li>Jens-Olaf Delfs, Institute of Geosciences, Christian-Albrechts-Universität zu Kiel, <i>Quantifying induced effects of subsurface thermal energy storage – the ANGUS project</i></li> <li>Shuang Chen, ENVINF, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Load shifting behavior in large-scale Borehole Heat exchanger (BHE) Array</i></li> <li>Boyan Meng, ENVINF, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Extensive utilization of shallow geothermal resources: A case study on a neighborhood in Cologne</i></li> </ul>
18:30	<b>Conference-Dinner and Get-together</b>		Foyer

**Wednesday, 9 October 2019**

09:00	<p><b>Session A3</b></p> <p style="text-align: right;"><b>Hall 1A</b></p>	<p><b>Session B3</b></p> <p style="text-align: right;"><b>Hall 1B</b></p> <p><b>09:00 – 12:30 (Coffee break included)</b></p>	
	<p><b>Conversion of surplus electricity to energy carriers and higher value chemicals (Power-to-X)</b></p> <p><b>Chair: Marcell Nikolausz</b></p> <ul style="list-style-type: none"> <li>• Simon Rittman, Department of Ecogenomics and Systems Biology, Universität Wien, <i>Highlights from ten years of pure culture biological CH<sub>4</sub> production from H<sub>2</sub>/CO<sub>2</sub></i></li> <li>• Washington Logroño, UMB, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>From surplus electricity and carbon dioxide to biomethane: The path with mixed cultures</i></li> <li>• Luis F.M. Rosa, UMB, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>MolkeKraft: From wastewater to jet fuel</i></li> <li>• Flávio C. F. Baleeiro, UMB, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>H<sub>2</sub> helps tackling electron donor scarcity during carboxylate chain elongation</i></li> </ul>	<p><b>Workshop Session: Decarbonizing urban heating and cooling systems</b></p> <p><b>Chair: Alena Bleicher, Sebastian Strunz</b></p> <p>Within this work-shop session we will identify research topics for interdisciplinary research on decarbonizing heating and cooling systems. UFZ-research in different disciplinary areas – economy, law, sociology, microbiology, monitoring technologies and modelling etc. – already contribute to this research field. However, it is advisable to bring researchers from the different disciplines at one table and develop research topics that can be addressed in an interdisciplinary manner.</p>	
10:30	<b>Coffee Break</b>		Foyer

11:00	<b>Session A 4</b> <b>Hall 1A</b>	<b>Continuation of Session B3</b> <b>Hall 1B</b>	
	<p><b>Photobiotechnology – Photosynthesis-driven H<sub>2</sub>-production</b></p> <p><b>Chair: Bruno Bühler</b></p> <ul style="list-style-type: none"> <li>• Jörg Toepel, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Redox biocatalysis and hydrogen production with phototrophic organisms</i></li> <li>• Sara Lupacchini, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Expression of the soluble oxygen tolerant hydrogenase from Ralstonia eutropha in Synechocystis</i></li> <li>• Samuel Grimm, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Improving H<sub>2</sub> production in the cyanobacterium Synechocystis sp PCC 6803</i></li> <li>• Franz Opel, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>Establishing a H<sub>2</sub>-sensing platform organism for the directed evolution of continuous, photosynthesis-driven H<sub>2</sub> production</i></li> <li>• Rohan Karande, SOMA, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, <i>From microbial community design to reactor engineering: linking diversity and dynamics for stable and continuous biocatalysis</i></li> </ul>	<p><b>Decarbonizing urban heating and cooling systems</b></p> <p><b>Chair: Alena Bleicher, Sebastian Strunz</b></p>	
12:30	<b>Lunch (individually)</b>		Canteen



## Keynote Speakers

### Professor Dr. Andreas Schmid, Department of Solar Materials, UFZ, Leipzig



Andreas Schmid is Head of the Department of Solar Materials and speaker for the topic 'Solar Fuels' in the Program Renewable Energies at the UFZ in Leipzig. He is professor for Biotechnology at the University of Leipzig since 2014. His main research areas are in the fields of photobiotechnology, single cell analysis, catalytic biofilms, redox biocatalysis and systems biotechnology. Previously Andreas Schmid was Chair of the Laboratory of Chemical Biotechnology in the Department of Biochemical and Chemical Engineering at the TU Dortmund University and Group Leader and Head of the 'Technical Enzymology' Laboratory, Institute of Biotechnology at the Swiss Federal Institute of Technology – ETH in Zurich. He is member on the Steering Committee Biotechnology Section at the Society for Chemical Engineering and Biotechnology and member on Board of Trustees at the Leibniz Research Centre for Working Environment and Human Factors. He is also member on the Advisory Board Biotransformation Section at the Society for Chemical Engineering and Biotechnology and Association for General and Applied Microbiology. He represents Germany on the Steering Committee of the European Federation of Biotechnology - Section on Applied Biocatalysis since 2002.

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### Prof. Dr. Daniela Thrän, Department of Bioenergy, UFZ, Leipzig



Daniela Thrän is Head of the Department of Bioenergy at the UFZ in Leipzig. She is also Head of the Bioenergy Systems Department at the German Biomass Research Centre (DBFZ) in Leipzig. She holds the chair for Bioenergy Systems at the University of Leipzig and is co-spokesperson for the "EnergyLandUse" integrated project in the Helmholtz "Terrestrial Environment" research programme. Daniela Thrän has been a member of the Bioeconomy Council since September 2012. She represents Germany on the ISO Committee "Biogenic Solid Fuels", is a member of the Energy Council for Saxony, coordinator of accompanying research for the "Biomass Energy Use" funding programme of the Federal Ministry for Economic Affairs and Energy (BMWi) and Head of Scientific Accompanying Research in the "Bioeconomy Cluster" (2012 - 2017). She has been working for two more years in the Extended Leadership Council of the Sustainable Development Solutions Network (SDSN) since January 2017.

# Abstracts

## Session A1: Workshop Session: Climate Change and its impact on renewable energy sources

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**Session coordinator and chairperson: Katja Bunzel<sup>1</sup>**

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<sup>1</sup> Department of Bioenergy, Helmholtz-Centre for Environmental Research – UFZ, Leipzig

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Renewable energy plays an important role in reducing greenhouse gas emissions and to mitigate climate change. However, the different renewable energy sources are also affected by climate change itself, via long-term changes in climate parameters, variability and extreme weather events. Mitigation and adaptation efforts might be hindered by that. Therefore, within this session, we want to discuss how we already incorporate these issues in our research and to identify open research questions.

**Venue:** Hall 1B

### **Schedule:**

<b>Time</b>	<b>Presentation</b>	<b>Speakers</b>
11:00 – 12:30	<i>Welcome Address and moderation</i>	Katja Bunzel (BEN)

## Session B1: Storage (and waste): Biogeochemistry of energy underground storage

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**Session coordinator and chairperson: Carsten Vogt<sup>1</sup>**

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<sup>1</sup> Department of Isotope Biogeochemistry, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany

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The German “Energiewende” policy is based on the establishment of green energy systems which are typically fluctuating and require an option for storage to compensate diurnal and seasonal variations. A key aspect of the “Energiewende” is to provide sufficient capacities for storing heat or renewable energy carriers, e.g. energy rich gases like methane or hydrogen, in underground reservoirs, which are considered to be safe, cost-efficient and sufficiently available. Assessment and monitoring of biogeochemical processes potentially occurring during storage of heat and energy carriers is crucial for the technical development as well as the social acceptance of underground storage reservoirs. While methane (in form of natural gas) has been successfully stored in pore or cavern storage facilities for decades in Germany and many other countries, the geological storage of hydrogen has not been focused on so far. Notably, the potential oxidation of hydrogen in reservoirs by lithoautotrophic microorganisms using different electron acceptors is an important but less studied aspect. Using aquifers for storage of heat is a promising technique for heating and cooling devices. Whereas several systems have been successfully operated at moderate temperatures (up to 25°C), the biogeochemical processes and ecological consequences associated with the storage of temperatures above 25°C are less understood. A new concept is to use polluted aquifers in urban areas for storage of heat, thus potentially accelerating natural attenuation (bioremediation) processes.

The safe phase-out of nuclear energy represents another significant aspect of the German “Energiewende” policy. The recently decided statutory selection procedure for a nuclear waste disposal site in Germany defines the requirement of comparing different disposal concepts in three internationally discussed host rock types (rock salt, crystalline and clay rock) aiming at the highest possible level of safety.

In session B1, current third party projects will be introduced focusing on characterizing biogeochemical processes associated with storage of gasses, heat, and nuclear waste.

**Venue:** Hall 1A

**Schedule:**

<b>Time</b>	<b>Presentation</b>	<b>Speakers</b>
<b>15:00 – 16:30</b>	<i>Welcome address</i>	Carsten Vogt (ISOBIO)
	<i>Biogeochemistry of hydrogen storage in salt caverns</i>	Laura Schwab (ISOBIO)
	<i>Tracking microbial hydrogen consumption by stable isotope tools</i>	Michaela Löffler (ISOBIO)
	<i>Biogeochemical effects of methane and heat in shallow aquifers – a field injection experiment</i>	Nina-Sophie Keller (ISOBIO)
	<i>Heat storage in polluted aquifers – killing two birds with one stone?</i>	Mohammad Sufian Bin-Hudari (ISOBIO)

## iCROSS - Integrity of nuclear waste repository systems - Cross-scale system understanding and analysis

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**Olaf Kolditz<sup>1</sup>**

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Co-Authors: Jörg Buchwald<sup>1</sup>, Nobert Grunwald<sup>1</sup>, Vanessa Montoya<sup>1</sup>, Florin Musat<sup>2</sup>, Thomas Nagel<sup>1,3</sup>, Renchao Lu<sup>1</sup>, Hans-Hermann Richnow<sup>2</sup>, Matthias Schmidt<sup>2</sup>, Haibing Shao<sup>1,3</sup>, Carsten Vogt<sup>2</sup>

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The interdisciplinary project iCROSS combines research competencies of five Helmholtz Centers in the topics of radiochemistry, geosciences, biosciences, geotechnical engineering and computational sciences, to contribute to the safe disposal of radioactive waste. Specifically, research concentrates to those host rock formations where the repository for high-level waste could be located according to the Site Selection Act – StandAG and where less research has been performed in Germany so far, i.e., clay and crystalline rocks.

Based on laboratory and in-situ test experiments, essential data is acquired, and parameters are derived for developing advanced modelling tools to gain a more profound process understanding from the molecular-, nano- up to the repository scales. In-situ test experiments are performed in large-scale underground research laboratories (URL) with focus on the Mont Terri site (CH; Opalinus clay), where under active involvement of German partners a new experimental gallery has been excavated. Further activities will take place in the Grimsel Test Site (CH; crystalline rock). Numerical methods for the analysis of thermal, hydraulic, mechanical and geochemical coupled processes in the Natural and Engineered Barriers are being developed specially, considering the existence of spatial heterogeneities in the system. These methods are implemented into the scientific open-source software OpenGeoSys-6, which ensures direct and efficient access by all developers and users within the context of joint programming. Laboratory experiments will be conducted to characterize biogeochemical processes affecting retardation and transport of radionuclides in geological clay section foreseen as nuclear waste repositories. Laboratory experiments obtained within the project are used to demonstrate the essential suitability of the developed methods, whereas in situ experiments form the basis for the definition and parametrisation of practice-oriented test examples and typical numerical benchmarks for model and software validation. This approach serves the development and validation of methods aimed at the envisioned cross-scale system understanding of the different interacting repository barriers.

The research leading to the results has received funding from the German Federal Ministry of Education and Research (BMBF, grant agreement 02NUK053A) and the Initiative and Networking Fund of the Helmholtz Association (HGF grant SO-093) within the iCross project.

## Biogeochemistry of hydrogen storage in salt caverns

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**Laura Schwab<sup>1</sup>**

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Molecular hydrogen is an energy rich compound. Being synthesized with excess renewable energy, it could be stored in underground salt domes as a backup for fluctuating energy and power demand. Due to their chemical and geotechnical properties, salt caverns seem to be very suitable as there is low chemical interference with the gasses stored and good isolation from outside contaminants. In Northern Europe, to date, salt caverns are used for long and short term storage of natural gas. But increasing temperatures have led to a reduced demand for gas and thus the existing caverns might easily be used for H<sub>2</sub> storage. H<sub>2</sub>, in contrast to CH<sub>4</sub> and CO<sub>2</sub>, is an excellent substrate for microorganisms. It is a molecular energy donor and electron shuttle that allows a diversity of metabolic processes depending on the electron acceptors present in the salt caverns. Anaerobic respiration processes can result in the formation of CH<sub>4</sub> or H<sub>2</sub>S coupled to H<sub>2</sub> oxidation. While the formation of methane is rather uncritical, elevated amounts of H<sub>2</sub>S can lead to corrosion and reduce the quality and chemical properties of the gasses stored. Research and knowledge on the physical and biogeochemical processes resulting from H<sub>2</sub> storage in salt caverns are scarce and the topic is only investigated through a few pilot projects worldwide. One such project is H<sub>2</sub>-UGS (H<sub>2</sub> Underground Storage) embedded in the HYPOS initiative, Hydrogen Power Storage & Solutions in East Germany in order to provide fundamental knowledge to launch a H<sub>2</sub>-Research Cavern in the future. Our research questions address the structure and function relationships of microbial communities present in caverns operated with natural and town gas and the impacts they can have on H<sub>2</sub> and H<sub>2</sub>/CH<sub>4</sub> caverns.



## Tracking hydrogenase activity with hydrogen stable isotope tools

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**Michaela Löffler<sup>1</sup>**

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Co-Authors: Steffen Kümmel<sup>1</sup>, Carsten Vogt<sup>1</sup>, Hans-Hermann Richnow<sup>1</sup>

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A hydrogen-based renewable power system requires storage of hydrogen (H<sub>2</sub>) in underground reservoirs. The potential oxidation of H<sub>2</sub> in such reservoirs by microorganisms is an important but less studied aspect.

Most microorganisms are equipped with at least one hydrogenase. Hydrogenases are a diverse class of enzymes catalyzing the reversible cleavage of molecular H<sub>2</sub> into two electrons and two protons. During H<sub>2</sub>-consumption the isotopic signature of the remaining H<sub>2</sub> changes. We tracked these changes in a study of a model organism, which uses the electrons of H<sub>2</sub> to reduce sulfate to sulfide. Our long-term goal is to develop a stable isotope tool based on changes in the isotopic signature of H<sub>2</sub> during oxidation by hydrogenases to detect and monitor potential biological losses during underground storage.

## Monitoring of the fate of methane injected into a pristine near-surface aquifer using stable carbon isotope analyses

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**Nina-Sophie Keller<sup>1</sup>**

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Co-Authors: Carsten Vogt<sup>1</sup>, Götz Hornbruch<sup>2</sup>, Ulrike Werban<sup>3</sup>, Hans-Hermann Richnow<sup>1</sup>

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A key issue of renewable energy concepts is the use of the underground for safely storing energy carriers like gases and heat, by utilizing, e. g., hydrogen (H<sub>2</sub>) or methane (CH<sub>4</sub>) in the Power-to-gas (PtG) process and aquifer thermal energy storage (ATES). Although CH<sub>4</sub> and H<sub>2</sub> are persistent in the deep anoxic reservoirs, as shown by long-time experience in many countries, effects of leakage incidents from gas pipelines or the ascent of gas from deep reservoir into near-surface areas are poorly understood. Furthermore, ATES performed at high temperature (up to 80 °C) or uncontrolled convection of heat energy induced by ATES in the subsurface could lead to adverse consequences on the drinking water resources in shallow aquifers. In this study, a field experiment was carried out to monitor the fate of methane which was injected into a pristine near-surface aquifer located near Wittstock/Dosse (Brandenburg, Germany). The conditions in the shallow underground may favor the microbial degradation of methane. Important questions are how - both aerobic and anaerobic - and how fast methane is degraded by microbes. A sensitive method for the monitoring of microbial methane losses in situ is compound specific stable isotope analysis (CSIA). Soil gas and groundwater samples were taken regularly before and after the injection and stable carbon isotope analyses of carbon dioxide (CO<sub>2</sub>) and CH<sub>4</sub> were conducted. The preliminary results show that methane ascended in soil and was degraded by microbes. The degradation took place preferentially in areas with sufficient oxygen available, i. e., in the unsaturated zone and at the edges of the gas plume. Dominant methane-oxidizing microorganisms are going to be characterized by molecular-biological methods.

## Biogeochemical effects of temperature changes on microbial communities and groundwater contaminations

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**Mohammad Sufian Bin Hudari<sup>1</sup>**

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<sup>1</sup> Department of Isotope Biogeochemistry, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany

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Aquifer thermal energy storage (ATES) is a means of renewable energy enabling the inter-seasonal heat storage and extraction from the subsurface. While operating temperatures typically range between 5°C and 20°C, temperatures of above 50°C are becoming increasingly commonplace. However, there have been concerns over impacts of elevated-temperature ATES situated in urban and industrial areas where anthropogenic sources of contamination are likely to be present. In normal ambient conditions, contaminants can be removed by natural attenuation under oxic or anoxic conditions by indigenous microorganisms. While it is believed that perturbations exceeding natural temperature variations may influence biodiversity and potential ecosystem services in the subsurface, their effects remain to be understood. This study explores how temperature changes may affect the biota in ATES systems and pollutant bioremediation in contaminated aquifers, to assess the limitations and effects of higher temperatures on population composition and its attenuation potential. We set up microcosms comprising sediments from pristine and contaminated aquifers spiked with <sup>13</sup>C-labelled substrates (e.g., toluene, acetate) and incubated at temperatures between 12°C to 80°C. Mineralization kinetics is determined by <sup>13</sup>CO<sub>2</sub> analysis, and stable-isotope probing (SIP) techniques are used to identify the responsible substrate-assimilating organisms. Preliminary results from one study consisting sediments from a contaminated site spiked with <sup>13</sup>C-labelled acetate under conditions at which sulfate is the main electron acceptor show that mineralization occurred at temperatures between 10°C and 80°C. However, after 36 days, analysis of <sup>13</sup>CO<sub>2</sub> showed that mineralization in setups incubated at, 45°C, 60°C, and 80°C seem to have stopped while complete mineralization was observed at 12°C, 25°C and 38°C. Amplicon sequencing data suggested that acetate was likely to be mineralized first by Alphaproteobacteria of the order Rhizobiales which are subsequently succeeded by several dominant anaerobic bacteria of the class Deltaproteobacteria, Anaerolineae and Clostridia once oxygen was depleted.

## Session A2: STROMER - Sustainable Transformation by Electrochemical Reactions

**Session coordinator and chairperson: Dr. Jens Krömer<sup>1</sup>**

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Rapidly expanding and fluctuating electric power production based on renewable sources creates a need for electricity storage and utilization. This offers unprecedented potential for the utilization of electric energy in environmental and bio-technology. In electrochemical systems electrons are used as a uniform equivalent to monitor, control and drive a wide diversity of different redox processes. Using electrons as process drivers in engineered systems, e.g. to synthesize value-added compounds or to degrade contaminants, fulfills the principles of sustainable chemistry and promises an unrivaled economic advantage. We develop unifying, applicable concepts for using electrochemical processes and reactors by controlling their inherent heterogeneities at different levels. By joining and strengthening existing capacities of different departments (ANA, ISOBIO, SOMA, TUCHEM, UBZ and UMB) at the UFZ we promote the formation of a leading cluster devoted to the research and application of electrochemical processes in environmental and bio-technologies. In the PhD college STROMER we aim at understanding and controlling electrochemical processes by unraveling and engineering the underlying heterogeneities to steer the process functions. STROMER includes four integrated PhD projects that are linked by the fundamentals of using electrons as universal currency for driving (bio)electrochemical reaction as well as the materials and methods used for their study

**Venue:** Hall 1A

### **Schedule:**

<b>Time</b>	<b>Presentation</b>	<b>Speakers</b>
<b>15:00 – 16:30</b>	<i>Welcome Address</i>	Jens Krömer (SOMA)
	<i>Carbon-based electrodes and electrode processes</i>	Jieying Zhou (TUCHEM)
	<i>Getting electrons in an out of cells</i>	Anh Vu Nguyen (SOMA)
	<i>Singles Species biofilms in bioelectrochemical systems</i>	Francesco Scarabotti (UMB)
	<i>Scaling (bio)electrochemical reactors</i>	Johannes Nelles (UBZ)

## Electrosorption of polar organic micropollutants on activated carbon-based materials

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**Jieying Zhou<sup>1</sup>**

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Being highly water-soluble and mobile, polar organic micropollutants (POMs) are increasingly detected in surface and groundwater, evoking potential threats to the environment and human health. Traditional water treatment strategies including adsorption by activated carbon materials fail to remove POMs efficiently due to their rather hydrophilic structures. Moreover, additional burdens on the environment are caused to regenerate the used activated carbon-based adsorbents in conventional ways, i.e. by transportation to facilities providing high-temperature regeneration. Electro-assisted sorption processes offer a clean, facile but promising solution to the removal of POMs on activated carbon-based electrodes and allow an easy on-site regeneration of the adsorbents. Previous studies focused mainly on exploring the electrosorption forces of activated carbon-based materials on inorganic ions (e.g. for capacitive deionization). In this work, the electrosorption of selected, differently charged POMs on conductive activated carbon felts (ACFs) that were modified with different surface functionalities was investigated. Our first results demonstrate that the ad-/desorption of the studied POMs is controllable by applying different potentials on ACFs. Selective removal of POMs carrying different charges is possible. Our work further studied the influence of the ACFs' surface chemistry on the electrosorption processes of target POMs. To analyze the ACFs, various characterization techniques were applied, including temperature-programmed desorption (TPD) to characterize O-containing functional groups, mass titration to determine the point of zero net proton charge and impedance spectroscopy as well as cyclic voltammetry to study the capacitance and the potential of zero charge. It was found that at the same polarization state, the adsorption of POMs is affected by the surface chemistry of the electrodes. Future work will aim at suggesting the best working conditions of the activated carbon-based electrodes for removal of POMs from water and on-site adsorbent regeneration.

## Getting electrons in and out of the cells: sugar catabolism of *Pseudomonas putida* KT2440 in bioelectrochemical reactor

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Anh Vu Nguyen<sup>1</sup>

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*P. putida* strain KT2440 is a promising microbial chassis for industrial applications due to its versatile metabolism, easiness of manipulation and high oxidative stress tolerance; however, the bacterium strictly relies on oxygen as terminal electron acceptor. Such aerobic metabolism is prone to oxidative carbon loss and cost-intensive reactor scale-up, compared to anaerobic processes. Bioelectrochemical systems (BES) provide an alternative way to remove electrons from catabolic reactions in the absence of oxygen by using an electrode, in combination with soluble redox mediators, as electron sink. In this study, we combine (bio)electrochemical analysis, metabolite analysis, and strain engineering to investigate the metabolic activity and possible internal limitations, of strain KT2440 under oxygen-free condition. Whereas preceding work has used glucose as substrate, by utilizing other carbohydrates as carbon inputs, we now aim to determine which carbon metabolic pathways are active and if the phenotype changes, when different sugar uptake systems can be used by the cells; this is combined with analyzing the energy and redox status of the cells under BES condition. Our preliminary results suggest that the periplasmic sugar oxidation pathway is mainly responsible for aldose metabolism and current production by KT2440 in BES, while energy yield and internal redox status are possibly still limiting factors. This finding paves the way for other possibilities of strain engineering that could help overcome those metabolic constraints, for instance, one that could improve redox mediator transport across outer membrane to increase energy production via periplasmic oxidation, or couple of the intracellular redox pools to membrane-bound oxidases via metabolic engineering.

## A closer look to the extracellular electron transfer in the model system *Geobacter sulfurreducens*

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**Francesco Scarabotti<sup>1</sup>**

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Co-Authors: Katja Bühler<sup>2</sup>, Christin Koch<sup>1</sup>, Falk Harnisch<sup>1</sup>

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Several dissimilatory metal-reducing microorganisms, such as *Geobacteraceae* are able to use a solid state electrode as terminal electron acceptor (TEA) of the respiratory chain. This mechanism is also known as extracellular electron transfer (EET). EET can be exploited in technical systems called microbial electrochemical technologies (MET). MET can be used, for example, to produce electrical current in microbial fuel cells by oxidizing the organic matter which is present in waste water. However the efficiency of this process and all other MET is still far from an industrial application.

In the last years the research interest is dedicated to the enhancement of MET and one important aspect to focus on is the elucidation of EET mechanism and thermodynamics and kinetics.

Here we exploit a tailor-made platform based on a fabricated microfluidic device and a transparent working electrode material, which enables noninvasive *real-time* monitoring of the electrical current with the number of cells attached on the electrode. Thus, the kinetics of the EET as well as the (averaged) current produced per single cell and the (averaged) yield coefficients can be analyzed.

Using the above described platform, this PhD project, within the frame of the STROMER\* ("sustainable transformation by electrochemical reactions") college, further aims to investigate the structure-function relationships between the electroactive species forming a biofilm (e. g. spatial distribution on the electrode and species abundance) comprising pure cultures and microbiomes and the influence of different operational parameters such as potential and applied flow rate on the performance of the system.

All the information achieved in this project will give the bases for future improvements of the EET and hence for engineering of MET.

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\* More information on STROMER available here: <https://www.ufz.de/index.php?de=44366>

## Scaling of electro(bio)reactors

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**Johannes Nelles<sup>1</sup>**

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Co-Authors: Steffi Hunger<sup>1</sup>, Luis Rosa<sup>2</sup>, Cristian Picoreanu<sup>3</sup>, Falk Harnisch<sup>2</sup>, Beate Strehlitz<sup>1</sup>

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The production of sustainable electric power production is expanding. However, electric power from renewable is fluctuating and decentralized and hence needs (new) technologies for storage and utilization. One possible technology platform for utilization of this energy is electrobiosynthesis. Here electrons are used via enzymes and microorganisms to drive and control processes allowing to produce a variety of chemicals such as e.g. platform chemicals or fuels. With these systems, a production and storage from excess electrical energy as sustainable energy carriers is possible via electro(bio)technological processes. Yet processes and operations to utilise renewable energy is still lacking. One reason for that is, that the development of electrobiotechnological processes in general needs knowledge-driven engineering which cannot be achieved using the existing and well established reactor technology. So far, the reactors used in electrobiosynthesis are mostly tailor made, non-optimised, or small and not scalable. Thus, a universal reactor platform is needed allowing the normalisation and standardisation of reactors and processes in electrobiosynthesis. This work is dedicated to the presents an approach for such an universal reactor platform and to identify the key influencing and scaling parameters on selected electrobiosyntheses. The work is based on an electro(bio)chemical upgrade kit for an infors multifors reactor<sup>1</sup>. Based on this and on a model in the computational fluid dynamics program “COMSOL Multiphysics” we aim to identify the limiting parameters of selected microbial electrobiosynthetic processes and electrobioreactors and find ways of opening the bottlenecks for scale up. Ultimately we aim on offering a blueprint for a reactor platform for electrobioreactor engineering and the following process optimisation.

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<sup>1</sup> Rosa, L.F.M., Hunger, S., Gimkiewicz, C., Zehnsdorf, A., Harnisch, F. (2017) Eng. Life Sci. 17 (1), 77 – 85



## Session B2: Modelling and numerical analysis of coupled multiphysics processes of geological thermal energy storage

**Session coordinator and chairperson: Haibing Shao<sup>1</sup>, Uwe-Jens Görke<sup>1</sup>**

<sup>1</sup> Department of Environmental Informatics, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany

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Although the provision of heating and cooling energy is by far the most important factor in a necessary transformation of the energy system, balanced and coordinated concepts for re-designing this energy sector are still lacking. Energy storage is an important component of the transformation of urban heating and cooling systems. Within the context of large-scale heat storage, the geological space plays a crucial role, since it offers large existing storage areas, which require a careful development, but can be managed in the sequence with relatively little effort.

Increasing interventions in the geological environment require careful analyses of the state of affected rock-fluid systems as well as of the feasibility, efficiency and environmental impact of storage considered technologies. A comprehensive understanding of the physical, geochemical and microbiological processes on all relevant time and length scales can only be obtained based on intensive laboratory and in-situ experiments combined with reliable studies in terms of modelling and simulation (numerical experiment) of the relevant processes.

This session addresses several aspects of the modelling of coupled processes of large-scale geological storage of thermal energy at different depths. Contributions are focused on computational process analysis and the evaluation of environmental impacts of geological energy storage.

**Venue:** Hall 1B

**Schedule:**

Time	Presentation	Speakers
17:00 – 18:30	<i>Welcome address</i>	Haibing Shao (ENVINF)
	<i>Overview Talk: Geoenergy Systems Analysis</i>	Jens-Olaf Delfs (Uni Kiel)
	<i>Load shifting behavior in large scale Borehole-Heat (BHE) exchanger (BHE) Array</i>	Shuang Chen (ENVINF)
	<i>Modelling the Aquifer-Thermal-Energy-Storage (ATES) in Hamburg</i>	Chaofan Chen (ENVINF)
	<i>Extensive Utilization of Shallow Geothermal Resources, a case study on a neighborhood in Kiel</i>	Boyan Meng (ENVINF)

## Quantifying induced effects of subsurface thermal energy storage – the ANGUS project

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**Jens-Olaf Delfs<sup>1</sup>**

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Co-Authors: Sebastian Bauer<sup>1</sup>, Christof Beyer<sup>1</sup>, Andreas Dahmke<sup>1</sup>, Jens-Olaf Delfs<sup>1</sup>, Johannes Nordbeck<sup>1</sup>, Bo Wang<sup>1</sup>

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New methods and technologies for energy storage are required for the transition to renewable energy sources. Subsurface energy storage systems such as salt caverns or porous formations offer the possibility of hosting large amounts of energy or substance. When employing these systems, an adequate system and process understanding is required in order to assess the feasibility of the individual storage option at the respective site and to predict the complex and interacting effects induced. This understanding is the basis for assessing the potential as well as the risks connected with a sustainable usage of these storage options, especially when considering possible mutual influences.

For achieving this aim, in this work synthetic scenarios for the use of the geological underground as an energy storage system are developed and parameterized. The scenarios are designed to represent typical conditions in North Germany. The types of subsurface use investigated here include gas storage and heat storage in porous formations. The scenarios are numerically simulated and interpreted with regard to risk analysis and effect forecasting. For this, the numerical simulators Eclipse and OpenGeoSys are used. The latter is enhanced to include the required coupled hydraulic, thermal, geomechanical and geochemical processes. Using the simulated and interpreted scenarios, the induced effects are quantified individually and monitoring concepts for observing these effects are derived.

This presentation will detail current activities concerning the design of geological thermal energy storages and the evaluation of their potential environmental impacts. The process implementation and numerical methods required and applied are detailed and explained. Application examples show the developed methods and quantify induced effects and storage sizes for the typical settings parameterized.

This work is part of the ANGUS2 project, funded by the Federal Ministry of Economic Affairs and Energy (BMWi) as part of the research initiative “Förderinitiative Energiespeicher”.

## Load shifting behavior in large-scale Borehole Heat exchanger (BHE) Array

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**Shuang Chen**<sup>1,2</sup>

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As a low-carbon technology of providing heating and cooling to buildings, utilizing shallow geothermal energy through Ground Source Heat Pump (GSHP) system is increasingly applied all over the world. A recent trend in the industry is to build large GSHP system targeting commercial buildings and small neighborhood. Such systems are typically constructed by connecting and linking hundreds of Borehole Heat Exchangers (BHE) through a pipe network. In such applications, the heat exchange rate of individual BHE is strongly dependent on the hydraulic and thermal processes in the pipe network.

In this study a comprehensive numerical model has been developed to simulate this coupling effect. Two existing open-source softwares, namely the finite element simulator OpenGeoSys, and the Thermal Engineering Systems in Python (TespY), are linked together in this work to simulate large GSHP system equipped with multiple BHEs. The model allows a dynamic heat extraction on individual BHE that is determined by the hydraulic process in the pipe network. The model is thus capable of capturing the long-term thermal interference among BHEs.

It is found that, the heat extraction rate on the centre BHEs was gradually shifted towards those located at the edge of the array in the long-term operation. Over different seasons, the strongest shifting phenomenon was observed in the month with the lowest thermal load. This becomes significant with the increasing number of BHEs installed in the array. As a result, traditional super-position based analytical approach is not accurate enough for long-term prognosis since it does not fully consider the thermal recharge and the thermal interference effects.

## Extensive utilization of shallow geothermal resources: A case study on a neighborhood in Cologne

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**Boyan Meng<sup>1</sup>**

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Utilization of shallow geothermal energy through ground source heat pump (GSHP) systems has become a well-established technology to provide heating and cooling in urban neighborhoods. However, the intensive exploration of geothermal heat within a limited area imposes high risks of system interaction. Hence, the quantitative assessment of long-term sustainability of high-intensity geothermal usage on the neighborhood scale is of great importance. This talk presents a case study using calibrated numerical models to evaluate the thermal impacts and predict the sustainability of intensive subsurface thermal use in a typical urban living quarter in Germany. The heat transport model was configured with site-specific parameters and validated against monitoring data. The heat pump performance was extrapolated from the simulated ground temperature profile. In addition, the effect of groundwater flow velocity was investigated under different advection scenarios. The results confirm the environmental and economical sustainability of the high-density GSHP applications at this particular site, largely due to the existence of a moderate groundwater flow regime. Furthermore, financial disadvantages are also anticipated due to efficiency losses of the heat pump, which are meant for the owners of the downstream installations. Analysis of thermal advection reveals the importance of hydrogeological investigations to achieve an optimal design and sustainable intensive use of shallow geothermal systems.

## Session A3: Conversion of surplus electricity to energy carriers and higher value chemicals (Power-to-X)

**Session coordinator and chairperson: Marcell Nikolausz<sup>1</sup>**

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Future energy systems worldwide will more rely on fluctuating renewable energy sources causing mismatches in production and consumption. Therefore, the major challenge of systems with high share of renewables is to store or utilize the surplus electricity. The Power-to-X concept has a broad meaning referring to the conversion of surplus electricity to products that can be used in other sectors. The session will mainly focus on biomethanation of hydrogen, which can be obtained by electrolysis of water. Grid quality methane can be used as fuel, chemical building block, carbon and energy source for single cell protein or bioplastics production, and it can be converted back to electricity. The other main focus of the session is to produce other higher value chemicals from hydrogen, such as medium-chain carboxylates or drop-in fuels, either via carboxylate chain elongation or by novel bioelectrotechnological processes utilizing also agricultural or agro-industrial wastes.

**Venue:** Hall 1A

### Schedule:

Time	Presentation	Speakers
09:00 – 09:05	<i>Welcome address</i>	Marcell Nikolausz (UMB)
09:05 – 09:30	<i>Highlights from ten years of pure culture biological CH<sub>4</sub> production from H<sub>2</sub>/CO<sub>2</sub></i>	Simon Rittman (Universität Wien)
09:30 – 09:50	<i>From surplus electricity and carbon dioxide to biomethane: The path with mixed cultures</i>	Washington Logroño (UMB)
09:50 – 10:10	<i>MolkeKraft: From wastewater to jet fuel</i>	Luis Rosa (UMB)
10:10 – 10:30	<i>H<sub>2</sub> helps tackling electron donor scarcity during carboxylate chain elongation</i>	Flávio Baleeiro (UMB)

## Highlights from ten years of pure culture biological CH<sub>4</sub> production from H<sub>2</sub>/CO<sub>2</sub>

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**Simon Rittmann<sup>1</sup>**

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Conversion of molecular hydrogen (H<sub>2</sub>), which may be obtained from various industrial flue gas sources or from surplus electricity, and carbon dioxide (CO<sub>2</sub>) to methane (CH<sub>4</sub>), is regarded as one of the keys enabling technologies for efficient and high rate renewable energy production and/or (renewable) power storage in Europe.

One of the available options for H<sub>2</sub>/CO<sub>2</sub> to CH<sub>4</sub> conversion is to utilize a pure culture of an autotrophic, hydrogenotrophic methanogen. A focus of our research was devoted to bioprocess development using the thermophilic archaeon *Methanothermobacter marburgensis*. Highlights from ten years of research on pure culture biological CH<sub>4</sub> production with *M. marburgensis* will be presented. An overview of closed batch, fed-batch, and continuous culture experiments from the last ten years of pure culture biological CH<sub>4</sub> production from H<sub>2</sub>/CO<sub>2</sub> using *M. marburgensis* will be given. Challenges, which were faced during bioprocess development, and in modelling results from already published biological CH<sub>4</sub> production experiments, will be discussed. Furthermore, results from a quantitative comparative physiological study using methanogens, and the development of high-pressure bioreactors, will be presented.

It is concluded that an efficient strain screening and selection procedure is necessary to prioritize the most productive autotrophic, hydrogenotrophic methanogens for the development of next generation high pressure pure culture biological CH<sub>4</sub> production bioprocesses.

## From surplus electricity and carbon dioxide to biomethane: The path with mixed cultures

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### Washington Logroño<sup>1</sup>

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Co-Authors: Sabine Kleinsteuber<sup>1</sup>, Denny Popp<sup>1</sup>, Paul Kluge<sup>1</sup>, Marcell Nikolausz<sup>1</sup>

<sup>1</sup> *Department of Environmental Microbiology, Helmholtz-Centre for Environmental Research – UFZ, Leipzig, Germany*

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Storing surplus electricity from wind power and photovoltaics is the current and future challenge for countries with massive renewable energy implementation. The problem can be technically addressed by chemical or biological conversion of hydrogen to methane using the Sabatier reaction or biomethanation, respectively. Biomethanation exploits the CO<sub>2</sub> reductive pathway of hydrogenotrophic methanogens to drive the conversion of electrochemically produced H<sub>2</sub> and CO<sub>2</sub> from various sources into CH<sub>4</sub>. Biomethanation by mixed cultures, which are envisioned as key biocatalytic resources for the future circular economy, will be presented as well as the advantages and disadvantages. Finally, microbial resource management was identified as a key concept for the selective biomethanation process. It is concluded that selective CH<sub>4</sub> production is possible by mixed cultures by selecting appropriate operational parameters and inoculum.

## MolkeKraft: From wastewater to jet fuel

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**Luis F.M. Rosa<sup>1</sup>**

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Co-Authors: Neubert Katharina<sup>1</sup>, Härtig Claus<sup>1</sup>, Falk Harnisch<sup>1</sup>

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Approximately 4 million tons of acid whey, a by-product of milk-processing industries, are produced in Germany annually. Yet, these cannot be exploited by existing technologies due to the composition and pH value. The treatment of the resulting waste water (with chemical oxygen demand (COD) > 70 g L<sup>-1</sup>) places high technological requirements and is characterized by a high energy demand. Mixtures of hydrocarbons, which can serve as fuel for combustion engines, are conventionally obtained from fossil resources. The most important obstacles for the use of renewable raw materials are the limited process efficiency, the "food versus fuel" discussion, and the CO<sub>2</sub> footprint of the entire value chain. Therefore, waste and wastewater are ideal resources for the sustainable production of chemicals and fuels.

The aim of the MolkeKraft project is to combine microbiological and electrochemical conversions to produce drop-in fuel for aviation, i.e. jet fuel, from acid whey on pilot scale.

MolkeKraft is the (German-based) acronym for microbial-electrochemical exploitation of sour whey for the production of drop-in aviation fuel a VIP+-project funded by BMBF (03VP06911 and 03VP06912) that is coordinated by the UFZ. The individual stages of the MolkeKraft process line were successfully demonstrated on laboratory scale in both, independent and joint preparatory work by the two affiliated partners, i.e. the Angenent lab (Tübingen University) and the Harnisch lab (UFZ).

The presentation will provide an overview on the concept of MolkeKraft and especially highlight the investigation and engineering of the electrochemical conversion.

See also: [www.ufz.de/molkekraft](http://www.ufz.de/molkekraft)



## H<sub>2</sub> helps tackling electron donor scarcity during carboxylate chain elongation

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**Flávio C. F. Baleeiro<sup>1</sup>**

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Anaerobic fermentation for carboxylate chain elongation is currently a hot topic due to its ability to convert agricultural and industrial waste streams into valuable medium-chain carboxylates (MCC) such as caproate and caprylate. The MCC yields in chain elongation are often limited by the amount of electron donors present in the waste stream (typically in form of lactate or ethanol). Through its role in the microbial metabolism and in thermodynamics, H<sub>2</sub> can act directly and indirectly as a supplemental electron donor for MCC production by mixed microbial communities. In future biorefinery schemes, H<sub>2</sub> together with a carbon source (e.g. CO<sub>2</sub>) can be used in anaerobic fermenters in order to support or become the main substrate for MCC production. Thus, the substrate spectrum of MCC production could be expanded widely, for instance on dry lignocellulosic biomass suitable for gasification. With that in mind, an overview of the state-of-the-art, as well as the challenges and perspectives of the concept will be given.

## Session A4: Photobiotechnology – Photosynthesis-driven H<sub>2</sub>-production

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**Session coordinator and chairperson: Bruno Bühler<sup>1</sup>**

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How can biotechnology contribute to the reduction of greenhouse gases in our atmosphere and to a decentralized energy supply? How can we produce energy sources and recyclables in an environmentally friendly and sustainable way from non-fossil resources? Which factors determine the efficiency and productivity of microorganisms as living catalysts and how can they product-oriented be maximized?

This session will discuss research at the Department of Solar Materials that addresses these questions with an integrated biotechnological approach combining expertise from systems bio(techno)logy, molecular biology, microbial physiology, biochemistry and process engineering. We focus on the development of new biotechnology concepts based on the principle of "bioartificial photosynthesis". These concepts exploit the natural ability of photoautotrophic cyanobacteria to split water using solar energy and simultaneously assimilate the greenhouse gas CO<sub>2</sub>. As a result, attractive products are formed: H<sub>2</sub>, which is intensively debated as a main fuel of the future fuel, and carbon intermediates, which can sustainably be converted via (partly artificial) microbial metabolic pathways into various chemical compounds. Up to date, these products are only produced in small quantities, and reaction systems are often unstable. Our goal is to produce these products in technically relevant quantities and to develop scalable photo-capillary bioreactors. The ultimate goal is the technically controlled realization of the biochemical "short circuit" - the generation of H<sub>2</sub> directly from water. This requires thorough investigation of the underlying biochemistry and cell physiology as well as of the determinants for catalytic efficiency. Resulting holistic understanding of the system will allow the design of powerful biocatalysts and technically scalable manufacturing processes, whose efficiency and sustainability can be quantified.

**Venue:** Hall 1B

**Schedule:**

<b>Time</b>	<b>Presentation</b>	<b>Speakers</b>
<b>17:00 – 18:30</b>	<i>Welcome address</i>	Bruno Bühler (SOMA)
	<i>Redox biocatalysis and hydrogen production with phototrophic organisms</i>	Jörg Toepel (SOMA)
	<i>Expression of the soluble oxygen tolerant hydrogenase from <i>Rastonia eutropha</i> in <i>Synechocystis</i> sp. PCC 6803</i>	Sara Lupacchini (SOMA)
	<i>Improving H<sub>2</sub> production in the cyanobacterium <i>Synechocystis</i> sp PCC 6803</i>	Samuel Grimm (SOMA)
	<i>Establishing a hydrogen-sensing platform organism for the directed evolution of continuous, photosynthesis-driven hydrogen production</i>	Franz Opel (SOMA)
	<i>From microbial community design to reactor engineering: linking diversity and dynamics for stable and continuous biocatalysis</i>	Rohan Karande (SOMA)

## Redox biocatalysis and hydrogen production with phototrophic organisms

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Cyanobacteria are promising organisms to be applied in biotechnological processes to produce chemicals or energy carriers such as H<sub>2</sub>. Prerequisites for efficient H<sub>2</sub> production with cyanobacteria are, beside the engineering of efficient and O<sub>2</sub>-tolerant hydrogenases, a deep understanding of the capacity and versatility of the photosynthetic apparatus. Electron balance analyses and the design of whole-cell redox biocatalysts enables us to characterize the potential of cyanobacteria to be exploited for H<sub>2</sub> production. Recently, oxygenase-based whole-cell biocatalysis has been realized in a photosynthesis-driven way within cyanobacteria. Thereby, oxygenases instead of hydrogenases function as an electron sink and specifically functionalized chemicals are produced. Phototrophic host organisms possess the advantage to provide both co-substrates of oxygenases, O<sub>2</sub> and activated electrons, via the light-driven photosynthetic water splitting reaction. Thereby, O<sub>2</sub> mass transfer limitation, a major bottleneck in O<sub>2</sub>-dependent biocatalysis, can be avoided. We present results on the application of different oxygenases for photosynthesis-driven oxyfunctionalization in the photoautotrophic cyanobacterium *Synechocystis* sp. PCC6803. For such strains, oxygenase-catalyzed reactions were shown to be light-dependent, in terms of both O<sub>2</sub> as well as electron supply. Quantitative physiological analyses of the photosynthetic apparatus showed the potential of cyanobacterial strains to be applied for redox biocatalysis. Electron balance analyses allowed us to determine the versatility of the photosynthetic apparatus to deal with electron and carbon sinks. The results revealed that the photosynthetic electron flux is enhanced under specific reaction conditions to provide electrons to artificial sinks (electron sinks, but also carbon sinks) without reducing carbon fixation for growth. The knowledge obtained will be applied in different strategies to produce H<sub>2</sub> with cyanobacteria. We will present approaches and first results utilizing an O<sub>2</sub>-tolerant hydrogenase in *Synechocystis* sp. PCC6803. The results of these studies provide a strong and promising basis for the future exploitation of photosynthesis for the efficient production of chemicals and H<sub>2</sub>.

## Expression of the soluble oxygen tolerant hydrogenase from *Ralstonia eutropha* in *Synechocystis* sp. PCC 6803

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Cyanobacteria are potential candidates to couple oxygenic photosynthesis to the production of molecular hydrogen (H<sub>2</sub>) using a bidirectional hydrogenase. They are regarded as promising “low-cost” microbial cell factories for a sustainable H<sub>2</sub> production. H<sub>2</sub> constitutes a high-energy fuel that burns cleanly in producing only water as its by-product. One of the major challenges in using native cyanobacterial hydrogenases is their high oxygen sensitivity. For this reason, our aim is to express the soluble oxygen tolerant NiFe-hydrogenase of *Ralstonia eutropha* in *Synechocystis* sp. PCC 6803. The active protein will be evaluated regarding H<sub>2</sub> production and consumption. Recently, the functional expression of the oxygen-tolerant hydrogenase from *R. eutropha* in *Synechocystis* has been achieved. Its characterization and optimization constitute the main focus of the project. We will present data regarding strain design, the evaluation of protein expression, and setups for activity tests. Finally, we will show analytic tools for the quantification of H<sub>2</sub> production and consumption under different growth conditions. Future research objectives include protein engineering, in order to improve the H<sub>2</sub> production capacity of the oxygen tolerant hydrogenase.

## Improving H<sub>2</sub> production in the cyanobacterium *Synechocystis* sp PCC 6803

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Recent reports of the Intergovernmental Panel on Climate Change (IPCC) on global warming, usage and exploitation of land, and marine resources demonstrate once more the need to implement and extend sustainable and climate-neutral product cycles. Since the use of fossil fuels largely contribute to CO<sub>2</sub> emission, new alternatives for renewable resources and energy carrier need to be discussed and evolved. Phototrophic microorganisms have the potential to function as biocatalyst for the CO<sub>2</sub>-based synthesis of high energy compounds by mainly using water and CO<sub>2</sub> for photosynthesis. By genetic engineering and optimization of growth condition, the cyanobacterium *Synechocystis* sp. PCC 6803 was shown to capable of producing a variety of valuable and energy-rich carbon compounds as well as H<sub>2</sub> as an energy carrier of the future. H<sub>2</sub> is produced by transferring electrons via metabolites or directly from the photosynthetic electron transport chain to hydrogenases. Most hydrogenases are inactivated by O<sub>2</sub>, limiting H<sub>2</sub> production by oxygenic phototrophic microorganisms. Also the native hydrogenase of *Synechocystis* is highly O<sub>2</sub>-sensitive. To obtain anaerobic conditions, expensive metal- or enzyme-based O<sub>2</sub> scavengers have been used, but their use on large scale is limited. New reactor designs are necessary to efficiently remove excess O<sub>2</sub> and products, control growth, and efficiently supply microbes with substrates (light and CO<sub>2</sub>). Growth of microbes in biofilm reactors led to enormous advantages including self-immobilization, self-repair, high cell density, and, in case of phototrophs, high light availability (Halan et al., 2012; Posten, 2009). Recently, a mixed-species capillary reactor design containing *Synechocystis* and *Pseudomonas* strains was shown not only to reduce O<sub>2</sub>-levels, but also to induce micro- and anaerobic conditions (Hoschek et al., 2019). Starting from this knowledge, mixed trophy biofilms were studied as a tool to improve H<sub>2</sub> production by *Synechocystis*.

- (1) Halan B., Bühler K. and Schmid A. Trends in Biotechnology, 2012, 30(9), 453-465
- (2) Posten C., Engineering in Life Sciences, 2009, 9(3), 165-177
- (3) Hoschek A., Heuschkel I., Schmid A., Bühler B., Karande R.\*, Bühler K. Bioresource Technology, 2019, 282, 171-178

## Establishing a hydrogen-sensing platform organism for the directed evolution of continuous, photosynthesis-driven hydrogen production

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Molecular hydrogen (H<sub>2</sub>) is believed to be an ideal candidate for future energy supply because it can be a clean, CO<sub>2</sub>-neutral energy carrier. Hence, a biotechnological production of H<sub>2</sub>, i.e., driven by photosynthesis, appears promising. A plethora of hurdles has however to be overcome to establish for instance a cyanobacterium as whole-cell biocatalyst for photosynthetic H<sub>2</sub> production. Therefore, my PhD project is designated to tackle that goal in a systematic way. In particular, we aim to establish a H<sub>2</sub> responsive regulatory cascade in the cyanobacterial model strain *Synechocystis* sp. PCC 6803 (*Synechocystis*). The natural H<sub>2</sub>-responsive system of the “Knallgas” bacterium *Ralstonia eutropha* positively regulates the transcription of two energy-generating uptake hydrogenases, which are only expressed at high level if H<sub>2</sub> is available under low energy abundance. This signal cascade comprises an oxygen-insensitive regulatory hydrogenase as H<sub>2</sub> detector of a two-component system, including a histidine kinase and a DNA-binding response regulator. These regulatory components will be transferred into *Synechocystis* and coupled with the expression of a reporter gene, namely the superfolder green fluorescent protein (sfGFP). Once *Synechocystis* expresses all the necessary components, a H<sub>2</sub>-dependent sfGFP fluorescence should be achieved. This biosensor can then be used for in vivo monitoring of H<sub>2</sub> and subsequently as tool for the systematic improvement of cyanobacterial H<sub>2</sub> evolution.

## From microbial community design to reactor engineering: linking diversity and dynamics for stable and continuous biocatalysis

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Solar energy is the most abundant source of energy available on this planet (1000-1400 W/m<sup>2</sup>), and it is considered to become a major energy source in the future. For effective utilization of solar energy, we need to understand and improve the efficiency of light capture, transfer, and storage. Nature provides us with excellent examples to convert solar energy, carbon dioxide, water, and other nutrients into organic carbon by utilizing microbial or plant photosynthesis. In plants, the structured design of a leaf combines the power of photosynthesis with miniaturization, microfluidics, and membrane separation concepts for maximizing solar energy to chemical energy conversion efficiency. In microbial mats, the activities of oxygenic and anoxygenic photoautotrophic as well as heterotrophic microorganisms are integrated for the effective utilization of solar energy. We investigate and make use of these concepts and their great potential to overcome current challenges in designing photo-biotechnological processes for the production of chemicals and energy carriers.

In this context, we will introduce biofilm (micro)reactors with a high surface to volume ratio (1333 m<sup>2</sup> m<sup>-3</sup>), enabling enhanced light availability and thus high cell densities (HCDs) of photoautotrophic microorganisms. However, oxygenic photosynthesis leads to O<sub>2</sub> oversaturation in such systems, impairing biofilm growth. We combined O<sub>2</sub> producing *Synechocystis* sp. with O<sub>2</sub> respiring *Pseudomonas* sp. and achieved HCDs of up to 51.8 g<sub>BDW</sub> L<sup>-1</sup> via such proto-cooperation.<sup>1,2</sup> This concept was coupled to the challenging C-H oxyfunctionalization of cyclohexane to cyclohexanol and enabled a remarkable conversion of >98% and a selectivity of 100% (KA oil). The HDCs enabled a productivity of 3.76 g<sub>cyclohexanol</sub> m<sup>-2</sup> day<sup>-1</sup>, which was stable for at least one month.<sup>3</sup> This mixed-species biofilm reactor platform currently also is applied for continuous H<sub>2</sub> production, utilizing synthetic microbial consortia that contain anoxygenic and oxygenic photoautotrophic as well as heterotrophic microorganisms.

- (1) Karande R., Hoschek A., Heuschkel I., Bühler K., Schmid A. Patent: PCT/EP2018/074746
- (2) Hoschek A., Heuschkel I., Schmid A., Bühler B., Karande R.\*, Bühler K. Bioresource Technology, 2019, 282, 171-178
- (3) Karande R., Salamanca D., Engesser K.-H., Buehler K. and Schmid A. Patent. WO/2018/046104



## Session B3/4: Decarbonizing urban heating and cooling systems – Urbane Wärmewende

**Session coordinator and chairperson: Alena Bleicher<sup>1</sup>, Sebastian Strunz<sup>2</sup>**

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### Workshop Session: Decarbonizing urban heating and cooling systems – Urbane Wärmewende

While the energy transition in the electricity sector is under way in Germany, little success has been achieved in the transport as well as in the heating and cooling sectors. To boost up the decarbonization of heating and cooling systems new approaches are necessary. Thus, questions on new technologies and their environmental impact have to be addressed – e.g. related to heat storage systems – as well as questions on how socio-cultural structures that shape patterns of heat consumption, and questions on the governance of the system. UFZ-research in different disciplinary areas – economy, law, sociology, microbiology, monitoring technologies and modelling etc. – already contribute to this research field. However, it is advisable to bring researchers from the different disciplines at one table and develop research topics that can be addressed in an interdisciplinary manner.

Taking up two events on the issue that took place earlier this year at the UFZ within this workshop session we will identify research topics for interdisciplinary research on decarbonizing heating and cooling systems.

**Venue:** Hall 2AB

#### **Schedule:**

Time	Presentation	Speakers
09:00 – 12:30	<i>Welcome address and moderation</i>	Alena Bleicher (SUSOZ) Sebastian Strunz (OEKON)