

# **MIMENIMA Summer school**

22.08. - 23.08.2018 in Etelsen

# "Mass transport in porous media with special consideration of imaging methods"





#### POROUS STRUCTURES – Where Science meets Application

Porous structures feature a large specific surface area that is crucial for catalysis and heat and mass transfer in various fields of technical application. The well-known Haber-Bosch process, being the foundation for nourish the world's population, is based on heterogeneous catalysis that would be impossible without porous substrates. But also in nature many environs like soil and rocks and objects such as plants and trees rely on porous structures. Their characteristics have to be taken into account in, e.g., mining, farming, and geothermal utilization.

Within the research training group MIMENIMA young researchers with different cultural and scientific background such as engineering, biology, chemistry, and material sciences work together on tailored novel porous ceramic structures for applications in energy supply, environmental and chemical processing, as well as space technology.

Inspiring talks from renowned experts in this summer school will give new impulses to identify scientific and technological key challenges for the next decade. The character of the symposium is informal and relaxed. We would like to give all participants the opportunity for open discoppenditions, to meet possible research partners, and to learn and adapte oncepts from other fields.

We wish you an inspiring and exciting meeting.

On behalf of the organizing board and all members of the research training group

Prof. Dr.-Ing. Kurosch Rezwan

Chairperson of MIMENIMA

#### MIMENIMA SUMMER SCHOOL

Mass transport in porous media with special consideration of imaging methods 22.08. – 23.08.2018 Etelsen / Germany

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22.08.2018	
09:30	Arrival and check-in
10:00	Welcome / Introductory comments
	Kurosch Rezwan and the organization board
10:30	Flash talks PhD
12:00	Lunch
13:00	Igor V. Koptyug
	Tomography Center
	SB RAS, Nowosibirsk
	"Magnetic resonance microimaging of catalysts
	and catalytic processes"
14:00	Coffee break and informal discussion
14:30	Muslim Dvoyashkin
	Institute of Chemical Technology,
	University of Leipzig
	"Molecular Diffusion in Functional Materials for
	Catalysis and Energy Storage – an NMR approach"
15:30	Informal sports programm
18:00	Barbecue
19:00	Evening Lecture
	Moritz Stefaner
	Truth & Beauty, Lilienthal
	"Beyond the bar chart: crafting information
	experiences"

23.08.2018	
09:00	Jan Kopyscinski Department of Chemical Engineering McGill University, Montreal <i>"In-situ spatial profiling of gas composition and</i> <i>catalyst surface temperature during highly exothermic</i> <i>reactions"</i>
10:00	Coffee break and informal discussion
10:30	Bernd R. MüllerDepartment of non-destructive testingBAM Federal Institute for Materials, Research and Testing,Berlin <i>"Microstructure characterization of materials using</i> X-ray refraction techniques"
11:30	Lunch
12:30	Moderated open discussion <ul> <li>cooperation</li> <li>open questions</li> <li>new visions</li> </ul>
14:00	Coffee break and informal discussion
14:30	Discussion of the project ideas in small groups
16:00	Presentations of the results
16:50	Closing remarks
17:00	Departure



# Participating Guest Speakers

Guest Speaker - Evening lecture

#### **Moritz Stefaner**

Self-employed Truth & Beauty Operator Lilienthal, Germany

mailto: moritz@stefaner.eu http://truth-and-beauty.net • http://datastori.es

#### Beyond the bar chart: crafting informati xperiences

Moritz Stefaner works as a "Truth and Beauty Operator" on the crossroads of data visualization, interface design and information aesthetics. He will walk us through a few of his recent explorations pushing the boundaries of data visualization — from visualizing wind predictions over cultural analytics to using food for representing data. At the heart of his work is the constant chase for the perfect shape of information — how

can we create unique, expressive, intriguing, and elegant data experiences?



#### **Guest Speaker**

#### Muslim Dvoyashkin

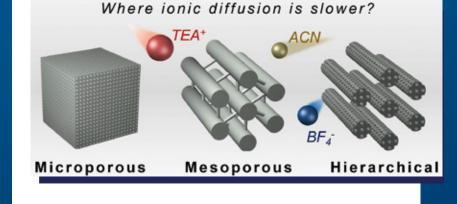
Dr., Junior Research Group Leader Institut für Technische Chemie Universität Leipzig



mailto: muslim.dvoyashkin@uni-leipzig.de https://itc.chemie.uni-leipzig.de/en/hc/

#### Molecular Diffusion in Functional Materials for Catalysis and Energy Storage – an NMR approach

The presentation focuses on molecular diffusion processes in a variety of nanostructured materials designed, e.g., for catalysis and energy storage applications, as seen by the pulsed field gradient NMR. In part, it will be discussed the nature of unexpectedly slow ionic transport in hierarchical model carbons for supercapacitors.







**Guest Speaker** 

#### Igor V. Koptyug

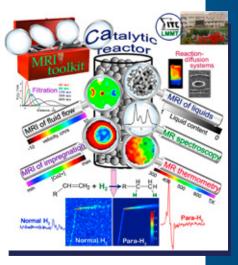
Prof. Dr. Sci., Deputy Director / Head of Laboratory International Tomography Center, SB RAS, Novosibirsk, RU



# Magnetic resonance microimaging of catalysts and catalytic processes

Magnetic resonance imaging (MRI) has become a powerful tool of modern medical diagnostics, while at the same time its applications in heterogeneous catalysis are relatively scarce. Nevertheless, thanks to the versatile nature of image contrast in MRI, the technique is not limited to morphological studies, but can also yield valuable parameter maps with a rich and diverse information content. The MR toolkit thus has a potential to provide a useful insight into heat and mass transport, phase transitions and chemical transformations, the key dynamic processes that govern a broad range of modern technologies. Examples to demonstrate include the MRI studies of the transport of solvents and solutes in porous materials during drying, sorption and supported catalysts preparation processes, as well as dynamic processes in catalysts and catalytic reactors during their operation. Yet, the major challenge in all such studies is the often insufficient sensitivity of NMR-based techniques, which is particularly severe in the MR studies that require imaging of gases.

Fortunately, an enhancement of NMR signals by several orders of magnitude is today's reality, with several ways to achieve this. One general approach



is based on the preparation and use of the samples with nuclear spin magnetization by far exceeding that in thermal equilibrium (spin hyperpolarization). In particular, nuclear spins can be hyperpolarized in a catalytic hydrogenation of unsaturated compounds with parahydrogen. Another possibility is to use the so-called remote detection NMR approach. Examples of the utilization of both approaches in catalytic MR studies will be presented. **Guest Speaker** 

#### Jan Kopyscinski

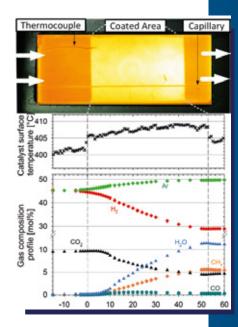
Prof. Dr., Assistant Professor Chemical Engineering McGill University, Montreal, Canada



# In-situ spatial profiling of gas composition and catalyst surface temperature during highly exothermic reactions

Modelling and optimization of chemical reactors require a good understanding of the reactions mechanism with the corresponding kinetic description. Therefore, high quality kinetic data are needed, which can be challenging to obtain, especially for fast and highly exothermic reactions such as the CO and  $CO_2$  methanation. Traditionally, kinetic studies rely on measuring the exit gas composition using differential reactors with diluted catalyst beds and reactants to avoid temperature change. In this talk an optically accessible catalytic channel reactor is presented that allows to gather spatially-resolved information on axial gas composition and catalyst surface temperature by means of a movable sampling capillary and short-wave infrared-thermography.

At the bottom of the channel reactor a catalyst coated plate is placed, while the top is closed with a set of two quartz glass plates for optically accessibility. Catalyst surface temperature determined via a



SWIR camera is not influenced by polyatomic molecules partaking in the reactions and thus do not falsify the kinetic data. In this work up to 60 data points per gas species can be collected for 1 experiment. The catalyst mass distribution along the reactor axis is determined using profilometry, enabling the development of a correct model for kinetic parameter estimation and model discrimination. **Guest Speaker** 

#### Bernd R. Müller



Dr., Senior Scientist /Deputy of Non-Destructive Evaluation (NDE) Department of non-destructive testing

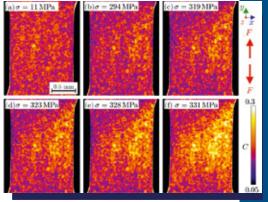
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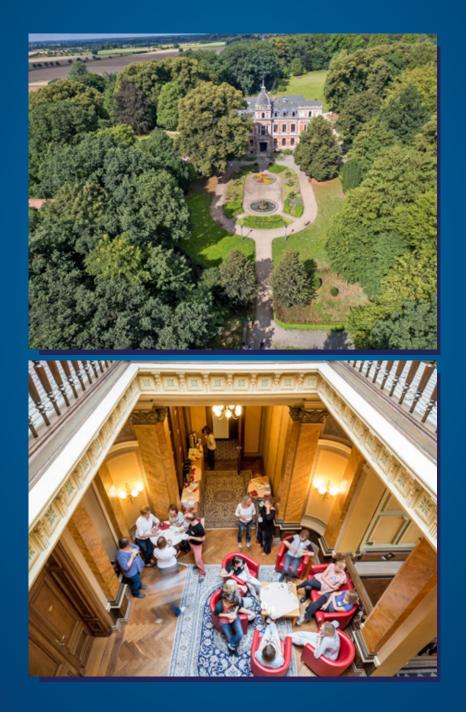
#### Microstructure characterization of materials using X-ray refraction techniques

X-ray imaging techniques have an enormous potential to understand the microstructure, its evolution, and its link to mechanical, thermal, and transport properties. In this lecture we report the use of a powerful, yet not so wide-spread, set of X-ray techniques based on refraction effects. X-ray refraction allows determining the internal specific surface of materials (surface per unit volume) in a non-destructive fashion, position and orientation sensitive, and with a nanometric detectability.

We demonstrate showcases of ceramics and composite materials, where microstructural



parameters could be achieved in a way unrivalled even by highresolution techniques such as electron microscopy or computed tomography. We present in situ analysis of the damage evolution during tensile load and the identification of void formation in parts produced by selective laser melting.



# PhD Students / Postdocs Flash Talks



#### **Thomas Ilzig**

"X-ray microtomography investigations of deep bed filtration process and their link to NMR-flow measurement."

Supervisors: St. Odenbach and W. Dreher



#### Mojtaba Mirdrikvand

"NMR methods for the characterization of mass transport and reaction processes in porous materials."

Supervisors: W. Dreher and M. Bäumer



#### Sangita Swapnasrita

"Simulation of catalytic reaction in porous structures and its optical characterization." Supervisors: Th. Wriedt and L. Mädler



### **Alex Schulz**

"Modeling of transport of rheological complex multiphase fluids in micropores and mircroporous membranes."

Supervisor: U. Fritsching and J. Thöming



#### **Ahmad Bakir**

"Determining three dimensional failure surfaces for porous ceramics from FE simulations and mechanical testing."

Supervisor: K. Rezwan and Th. Hochrainer



## Mehrdad Sadeghi

"Mass transport in graded monolithic catalysts during gas and multiphase reactions." Supervisors: J. Thöming and U. Fritsching



#### Malte Lorenz

"Investigation of dielectrophoretic effects in porous structures."

Supervisors: M. Baune and J. Thöming



## Karoline Gajda

"Inorganic foam structures by using residual materials ."

Supervisors: J. Thöming and K. Rezwan



#### Marieke Hoog Antink

"Proteolytic ceramic capillary membranes for the preparative production of bioactive peptides."

Supervisors: M. Maas and K. Rezwan



# Dr. Jana Markhoff

"Protein Adsorption on Meso- Macroporous Ceramics."

Supervisors: D. Brüggemann and K. Rezwan



### Jessica C. Mainardi

"Porous ceramic nanocomposites with embedded biofunctionality." Supervisors: M. Maas and K. Rezwan



#### **Thamires Silva**

"New polysiloxanes-based electrode materials for Microbial Fuel Cells (MFCs)." Supervisors: M. Wilhelm and K. Rezwan



#### **Vignesh Ahilan**

"Preparation of Porous Ceramic Membranes for Integrated Microbial Fuel Cell – Membrane Bio Reactor (MFC - MBR)."

Supervisors: M. Wilhelm and K. Rezwan



#### Dr. Sarabjeet Kaur

"Synthesis and Fabrication of SiC – based Ceramic Nanocomposites Foams with Micro-Meso-Macroporosity." Supervisors: M. Wilhelm and M. Bäumer



#### Dr. Prabu Moni

"Synthesis of Multifunctional Hybrid Ceramics derived from Polysiloxanes for Electrochemical Applications."

Supervisors: M. Wilhelm and K. Rezwan



## **Daniel Schumacher**

"Multifunctional precursor derived ceramics prepared by freeze casting technique." Supervisors: M. Wilhelm and M. Dreyer



#### **Dawid Zimnik**

"Application of porous ceramics for the handling of cryogenic media in space." Supervisors: M. Dreyer and M. Wilhelm

#### PARTICIPANTS

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MIMENIMA Summer school

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