MIMENIMA

Graduiertenkolleg
GRK 1860

MIMENIMA Symposium

28.09. - 30.09.2015 in Grömitz

Baltic Coast

”Porous Structures -
Where Science meets Application“

Universität Bremen*

*EXCELLENT.

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 like 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.

During the symposium we bring together people from industry and science under the central topic of porous structures. In the enjoyable atmosphere of the Baltic Coast we would like to discuss established concepts and develop new ideas regarding characterization, description, and application of porous media. Inspiring talks from renowned experts 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 like to give all participants the opportunity for open discussions, meeting possible research partners, and learning and adapting concepts 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 SYMPOSIUM
Porous Structures – Where Science meets Application
28 – 30 September 2015
Grömitz / Germany

28.09.15	
12:30	Arrival and check-in
12:30 – 01:30	Lunch
01:30 – 02:00	**Welcome / Introductory comments by the speaker and the organization board** **Kurosch Rezwan**
Session 1 (Chair: Lars Kiewidt)	
02:00 – 02:45	**Gerhard Mestl** Department Oxidation Catalysis, Clariant AG, Heufeld, Germany ***"Catalysis in industrial application"***
02:45 – 03:00	Coffee break
03:00 – 03:45	**Edward J. Garboczi** Applied Chemicals and Materials Division Material Measurement Laboratory, National Institute of Standards and Technology (NIST), Boulder, USA ***"X-ray tomography, spherical harmonics, and finite elements: Understanding random particles and materials"***
03:45 – 04:00	***"Future challenges in porous media – Impulses for open discussion"*** **Kurosch Rezwan**
04:00 – 04:30	Coffee break
04:30 – 06:30	**Open discussion**
06:30	Dinner

29.09.15	
07:00 – 09:00	Breakfast
09:00 – 09:15	Résumé of day 1 and outlook on day 2 **Kurosch Rezwan**
Session 2 (Chair: Laura Luhede)	
09:15 – 10:00	**Marc-Olivier Coppens** Department of Chemical Engineering, University College London, U.K. ***"Nature-Inspired Design and Synthesis of Porous Materials for Catalysis, Separations and Biomedical Applications"***
10:00 – 10:15	Coffee break
10:15 – 11:00	**Adam Lee** European Bioenergy Research Institute (EBRI) Aston University, Birmingham, UK ***"Hierarchical Catalyst Architectures for Sustainable Chemical Transformations"***
11:00 – 12:30	**Open discussion**
12:30 – 01:30	Lunch
Session 3 (Chair: Benjamin Besser)	
01:30 – 02:15	**Inga Berre** Department of Mathematics, University of Bergen, Norway ***„Flow and permeability enhancement in fractured geothermal reservoirs"***
02:15 – 02:30	Coffee break
02:30 – 03:15	**Krishna M. Pillai** Department of Mechanical Engineering, University of Wisconsin-Milwaukee, USA ***"Use of sharp interfaces in flow models to predict wetting of industrial porous media"***
03:15 – 03:30	***"Future challenges in porous media – Intermediate results"*** **Kurosch Rezwan**
03:30 – 04:30	**Open discussion**
04:30 – 05:30	Sports, events (e.g. Cricket, Beach Volleyball) and group foto
06:00 – 07:30	Dinner
07:30 – 08:30	Special Event blond & bieber, Rasa Weber

30.09.15	
07:00 – 09:00	Breakfast and check-out
09:00 – 09:15	Résumé of day 2 and outlook on day 3 **Kurosch Rezwan**
Session 4 (Chair: Thomas Veltzke)	
09:15 – 10:00	**Martin Dieterle** BASF Ludwigshafen, Germany ***"Shale Gas Opportunities: Alkane Activation"***
10:00 – 10:15	Coffee break
10:15 – 11:00	**Rainer Helmig** Department of Hydromechanics and Modelling of Hydro systems, University of Stuttgart, Germany ***"Modelling and analysis of mass, momentum and energy-transfer processes at the interface between free and porous-media systems"***
11:00-12:15	**Open discussion**
12:15-13:00	**Résumé of symposium, lessons learned, open questions** **Kurosch Rezwan**
13:00-14:00	Lunch
14:30	Departure

Participating Guest Speaker

in Alphabetical Order

Guest Speaker

Inga Berre

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University of Bergen
Bergen, Norway

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Short CV

Berre is Professor in the Porous Media Group at the Department of Mathematics, University of Bergen Norway. She also holds a position as scientific advisor at Christian Michelsen Research. She is chair of the board for the Norwegian Centre for Geothermal Energy Research and member of the Board for the Division of Science, Research Council of Norway. Berre has lead several research projects related to modeling and simulation of flow and transport in subsurface porous media, and is currently leading the projects GeoStim and FracZone.

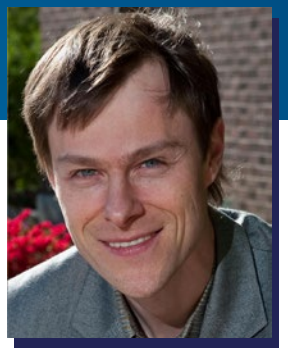
Research area

Berres research interests are efficient numerical methods for simulation of flow and transport and the solution of parameter identification problems in porous media, the last years mainly motivated by achieving better understanding of processes in fractured reservoirs. Currently, a particular interest is on modeling and simulation of permeability enhancement of fractured geothermal reservoirs.

abstract (talk)

Flow and permeability enhancement in fractured geothermal reservoirs

Enhanced geothermal systems (EGS) technology can enable geothermal energy production in regions where it is otherwise not commercial. In formations where the differences between maximum and minimum horizontal in-situ stresses are large and natural fractures already exist, which is typical where EGS is considered, the most efficient mechanism of stimulation is not propagation of tensile cracks away from the wellbore, but rather shear displacements improving the permeability of existing fracture networks. We give an overview of relevant physical processes and fracturing mechanisms as well as challenges related to upscaling and simulation of flow and shear-dilation in fractured reservoirs. A discrete fracture-matrix model for simulation of flow and the shear-dilation in a fractured media for a low-pressure stimulation scenario is proposed. Considering fractures as hybrid lower-dimensional elements in space for the flow simulations facilitates handling of dynamic fracture apertures.



Guest Speaker

Marc-Olivier Coppens

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Short CV

Ramsay Memorial Professor and Head of Department of Chemical Engineering at University College London (UCL), since 2012. MSc (1993) and PhD (1996) degrees in chemical engineering from Ghent University in Belgium; postdoctoral fellow at Yale and UC Berkeley; at TU Delft from 1998-2006, where he became van Leeuwenhoek Professor in Reactor & Catalysis Engineering in 2001 and Chair of Physical Chemistry and Molecular Thermodynamics in 2003. He was a Professor at Rensselaer (RPI), USA, from 2006-2012. At UCL, he is also Director of the Centre for Nature Inspired Engineering – one of five, 5M£ "Frontier Engineering" Awards by the UK's National Science Foundation, EPSRC. Won numerous international awards, published over 100 peer-reviewed journal publications to date, and presented more than 50 keynote and plenary lectures. Fellow of the IChemE, the first International Director of the AIChE's CRE Division, and active on AIChE's International Committee and Particle Technology Forum.

Research area

Professor Coppens' research centers on Nature-Inspired Chemical Engineering (NICE), that is, to design and realize efficient chemical reaction processes, porous catalysts, and separation systems, guided by the fundamental mechanism underlying desirable properties, like scalability and robustness, in biological systems, from molecular to macroscopic scales. Applications are in the areas of resource efficiency (energy, water and materials), sustainable chemical production, and health.

abstract (talk)

Nature-Inspired Design and Synthesis of Porous Materials for Catalysis, Separations and Biomedical Applications

My presentation will discuss how we can take guidance from two prevalent mechanisms in biological systems to design better porous materials for a range of valuable applications in catalytic reaction engineering, energy and health. These mechanisms are force balancing via confinement in nanopores (such as in chaperones and aquaporins), and scalability via hierarchical transport networks with optimized geometry (such as in trees and lungs). Rather than mimicking nature, we seek to understand the fundamental mechanisms behind desirable traits, and apply these in the context of engineering applications. This nature-inspired chemical engineering (NICE) approach involves analytical theory and computer simulations to support design and synthesis of porous catalysts, membranes, fuel cells and materials for controlled drug delivery.

Guest Speaker

Martin Dieterle

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Short CV

Martin Dieterle studied chemistry at the TU-Berlin and did his PhD at the Fritz-Haber institute. Since 2001 he is working within BASF Research on the development of heterogeneous catalysts. Initially he worked in the area of alkane dehydrogenation and selective oxidation. Since 2007 he managed a group in the USA for the development of catalysts for selective catalytic reduction (SCR) in exhaust gas treatment. Since 2010 he is leading a group for the development of petrochemical catalysts in Ludwigshafen.

abstract (talk)

Shale Gas Opportunities: Alkane Activation

Historically the main source of alkane activation to higher olefins, e.g. propene and butenes, has been the steam cracker, as ethylene co-product. Traditionally, naphtha has been the main feedstock for steam crackers. The discovery and use of shale gas in North America has become a game changer for the chemical industry by providing access to cheaper and lighter fossil feedstocks. At the same time the growth in demand of higher olefins is expected to exceed that of ethylene in the coming decades. The increased number of crackers using a lighter feedstock coming on stream triggers interest in alternative on purpose alkane activation technologies to produce higher olefins. Current research topics related to alkane activation including dehydrogenation, dehydroaromatization (Methane to Benzene) and dry reforming will be discussed.

Second part: Industrial requirements of catalysts development

Guest Speaker

Edward J. Garboczi

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Short CV

Dr. Edward Garboczi is a Fellow in the Applied Chemicals and Materials Division at the National Institute of Standards and Technology (NIST), Boulder, Colorado, USA.

Dr. Garboczi is a member of the American Physical Society, a Fellow of the American Ceramic Society and the American Concrete Institute, and a member of RILEM. He received the 1992 RILEM Robert L' Hermite Medal, a 2009 NIST Silver Medal, the 2009 Edward Henry Award and the 2012 Della Roy Lecture Award from the American Ceramic Society, and the 2014 Robert Philleo Award from the American Concrete Institute.

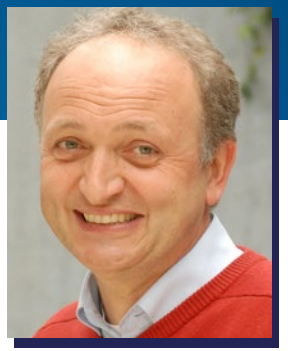
Research area

Dr. Garboczi's main research is on the computational materials science of particle-based composite materials, using computer-based microstructural models and X-ray computed tomography (CT) images along with numerical algorithms. Materials include ceramics, metals, foams, and cement-based materials, and percolation and composite theory are used to interpret numerical results. Because 3D particle shape is important for composites and many other areas of application, Dr. Garboczi uses X-ray CT and spherical harmonic analysis to build quantitative mathematical models of random-shaped particles, with applications to lunar soil, chemical explosives, concrete, and tumors.

abstract (talk)

X-ray tomography, spherical harmonics, and finite elements: Understanding random particles and materials

Techniques such as X-ray computed tomography (CT) allow one to image the interior of random materials and determine the phase structure. Numerical algorithms such as the finite element technique then allow computations of properties to be made directly on the measured structure. This combination of theory and experiment, in conjunction with analytical composite and percolation theory, then enables quantitative, theoretically sound microstructure-property relationships to be formulated. X-ray CT, in combination with spherical harmonic analysis, enables quantitative shape measurement of the particles that are often the basis of microstructure. True three-dimensional particle shape analysis has many other applications as well. Illustrations of these kinds of research will be given in the fields of concrete, polymer foams, metallic additive manufacturing, and lunar soil composites.



Guest Speaker

Rainer Helmig

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of Hydrosystems
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Short CV

2 / 1993	Doctoral degree (Dr.-Ing.), University of Hannover
1993 – 1997	Research assistant, Institute of Hydraulic Engineering, University of Stuttgart
11 / 1996	Habilitation degree (Dr.-Ing. habil.), University of Stuttgart
1997 – 1998	Acting Professor for Numerical Methods and Information Processing at the Institute of Computer Applications in Civil Engineering, TU Braunschweig
1998 – 2000	Full Professor for Numerical Methods and Information Processing at the Institute of Computer Applications in Civil Engineering, TU Braunschweig
since 2000	Full Professor of Hydromechanics and Modelling of Hydrosystems and Director, Institute for Modelling Hydraulic and Environmental Systems, University of Stuttgart

Research area

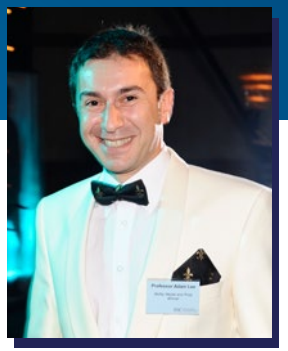
Rainer Helmig' s research interests are related to multi-phase physics in porous media, the development of thermodynamically consistent model concepts and their transfer to robust and efficient numerical schemes. These models are applied to environmental problems such as CO_2 storage and energy storage in the underground; the influence of these applications on groundwater is also a focus of our research. In the last five years, the modeling and analysis of soil-moisture processes in the subsurface, and especially the influence of evaporation and salt precipitation in groundwater has become a central topic of research.

abstract (talk)

Modelling and analysis of mass, momentum and energy-transfer processes at the interface between free and porous-media systems

Flow and transport processes in domains composed of a porous medium and an adjacent free-flow region appear in a wide range of industrial, environmental and medical applications. In this context, evaporation is a ubiquitous process, since evaporation rates and patterns affect the energy balance of terrestrial surfaces and drive an array of climatic processes. Notwithstanding its prominence for many natural and engineering applications, the prediction of evaporative drying rates from porous media remains a challenge due to complex interactions between the porous-medium and the free-flow system, the ambient conditions (radiation, humidity, temperature, air velocity, turbulent conditions) at the interface, and the internal porous-medium properties that lead to abrupt transitions and rich flux dynamics.In this lecture, we will:

- explain the relevant processes of mass, momentum and energy transfer at the interface between a free-flow and a porous-media system;
- provide a new coupling concept for modelling coupled porous-medium and free flow with application to evaporation and salt-precipitation processes. A comparison study will show the advantages and disadvantages in comparison with classical approaches;
- introduce three model combinations for evaporation processes and employ them to study the effects of various quantities and processes: a porous-medium model coupled with a laminar free-flow model, with a simple boundary-layer model, and finally with a Reynolds-averaged turbulence model which uses algebraic expressions to account for the turbulent flow behaviour. These model combinations are employed to evaluate the influence of different parameters and processes on the computed drying rates. The results will be compared and discussed with experimental measurements on different scales;
- present various numerical examples that will illustrate the influence of soil-moisture processes in the subsurface on the groundwater budget and quality.



Guest Speaker

Adam Lee

European Bioenergy Research Institute
Aston University
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Short CV

Adam Lee is Professor of Sustainable Chemistry and an EPSRC Leadership Fellow in the European Bioenergy Research Institute, Aston University. He holds a BA and PhD from the University of Cambridge, and has held Chair appointments at Cardiff, Warwick and Monash universities. His research addresses the rational design of nanoengineered materials for clean catalytic technologies, and the development of in-situ methods providing molecular insight into surface reactions, for which he was awarded the 2012 Beilby Medal and Prize by the Royal Society of Chemistry. He has published >150 peer-reviewed articles (H-index 38) and is a FRSC, AFIChemE, MRACI and serves on several journal editorial boards.

Research area

Catalysis is a core area of science and technology and key contributor to the global economy (>$10 trillion annually), with the potential to transform society through addressing diverse topics spanning energy, climate change, health and sustainability. Key challenges facing catalysis are (i) the lack of fundamental molecular level insight into structure-function relations and reaction mechanisms that dictate ultimate macroscopic performance, (ii) the need for new methodologies to control the nature, distribution and robustness of practical catalysts, and (iii) the discovery of new sustainable chemical transformations employing renewable resources.

abstract (talk)

Hierarchical Catalyst Architectures for Sustainable Chemical Transformations

The quest for sustainable technologies to meet the food, energy and material challenges of this century is a key driver for the design of next-generation catalysts and industrial chemical processes. Chemoselective oxidations and hydrogenations of alcohols and carbonyls respectively, and (base)acid catalysed (trans)esterifications, are important reactions that underpin the synthesis of diverse chemical intermediates, and will play a key role in the valorisation of biomass for the production of biofuels and bio-derived chemicals. Unfortunately, current heterogeneous catalysts are poorly suited to the chemical transformation of bulky reactants, such as lignocellulosic components or oleochemicals from plants or algae, or rapid molecular transport of reactants/products to and from in-pore catalytically active sites. New synthetic methodologies are therefore required to improve the accessibility and connectivity of porous catalyst architectures.

Here we highlight how advances in inorganic synthetic protocols afford the rational design of mesoporous and hierarchically ordered macroporous-mesoporous architectures for aerobic selective alcohol oxidations and the transformation of bio-derived feedstocks for the sustainable production of biodiesel and chemical intermediates for the polymer, fragrance, flavourings and pharmaceutical sectors.

Guest Speaker

Gerhard Mestl

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Short CV

- Since 7/2006 Department Head, Oxidation Catalysis, Clariant AG (Süd-Chemie AG), Heufeld
- 2/2005-6/2006 Project Manager, PA-Catalysts, Süd-Chemie AG, Heufeld
- 2/2002-2/2005 Chief Technology Officer, NanoScape AG, Munich,
- 08/2001 – 11/2001 Visiting Associate Professor at the ECPM of the CNRS at Strasbourg, France (Director Prof. M Ledoux), 2001. “Multiwalled Carbon Nanotubes for Partial Oxidation Reactions.”
- 6/1997-6/2002 Head of Research Group „Heterogeneous Catalysis“, Department of Inorganic Chemistry, Fritz-Haber-Institut der Max-Planck Gesellschaft (Director Prof. Dr. R. Schlögl), Berlin, Germany. “Mixed Metal Molybdates, Heteropoly Acids, Ag- and Cu- Catalysts, and Multiwalled Carbon Nanotubes for Partial Oxidation Reactions.”
- 1/1996 - 6/1997 Feodor-Lynen Research Fellowship of the Alexander-von-Humboldt Foundation, Department of Chemistry, Texas A&M, College Station, TX., USA, (Prof. J. H. Lunsford). “In Situ Raman Spectroscopic Characterization of NO-Decomposition over Ba-Catalysts.”
- 9/1994 - 12/1995 Head of Research Group „Catalysis“, Department Surface Chemistry and Catalysis, (Prof. R. J. Behm), University of Ulm, Germany. “Pd on Atomically Flat Quartz, Sapphire, Rutil and HOPG as Models for VAM-Catalysts.”
- 7/1990 - 7/1994 Ph.D. Thesis “Raman spectroscopic Characterization of Oxide Catalysts.” (LMU, advisor Prof. H. Knözinger).

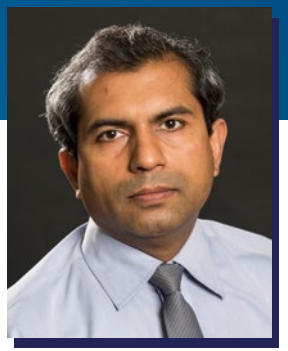
Research area

Heterogeneous catalysis contributes to virtually every technical product in one way or the other. Its economic importance hence cannot be overestimated. Therefore, there is a constant drive for the development of more improved catalytic processes and of course catalysts too. Our department is focusing on the development of heterogeneous selective oxidation catalysts for all major industrial applications.

abstract (talk)

Catalysis in Industrial Application

Catalytic selective partial oxidation reactions have one major challenge: in the thermodynamic equilibrium, CO_2 would be the only product formed. The catalysts and the catalytic processes therefore have to be designed such that thermodynamically unstable intermediates are formed in maximum yields. Of course the design of the catalytic surface itself - the active centers - plays an important role in this context as well as the process design by the chemical engineers. But even the optimum catalyst surface under optimum reaction conditions will lose all its advantages if the contact time of the reactants with the surface is in the wrong regime. CO_2 will then only be formed, or the reactants will be insufficiently converted. Therefore, the tailoring of the pore system, reacting pores and transport pores as well, of a heterogeneous catalysts to the respective catalytic reaction is of very high importance for optimum performance.



Guest Speaker

Krishna M. Pillai

Laboratory for Flow and Transport
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Short CV

Dr. Krishna M. Pillai is an Associate Professor in the Mechanical Engineering Department at University of Wisconsin-Milwaukee (UWM), USA. He is also the director of Laboratory for Flow and Transport Studies in Porous Media at UWM.

Dr. Pillai received his B.Tech. and M.Tech. degrees from the prestigious I.I.T. Kanpur of India. He did his Ph.D. from University of Delaware, USA under Prof. Suresh Advani and later completed a post-doctoral research fellowship under Prof. Chuck Tucker III of University of Illinois, Urbana-Champaign, USA.

Research area

Dr. Pillai's research interests span several fields of porous media including processing of composites, wicking of liquids, evaporation of multicomponent liquid mixtures, and oil exploration. He has published extensively in reputed journals and presented his work in numerous international conferences and workshops. He is a co-editor of the book 'Wicking in Porous Materials'. He is in the editorial boards of two prestigious international journals including Composites Part A, and is also a member of the scientific committee for the FPCM (Flow Processes in Composites Materials) conferences. He was a laureate of the 2014 Rosette award by Interpore, the international society for porous media research, for organizing its 2014 annual conference. Several multinational companies, state agencies, as well as the National Science Foundation (NSF) of USA have funded Dr. Pillai's research. He was awarded the prestigious CAREER grant in 2004 by NSF.

abstract (talk)

Use of sharp interfaces in flow models to predict wetting of industrial porous media

In several industrial applications such as manufacture of composite materialsor dispersal ofincense through wicks or dyeing of textiles, it is often important to completely wet a porous substrate with a liquid. In many such applications,the flow of the wetting liquid inporous media is led by a sharpliquid-front. In order to optimize such wetting processes, the flow model based on Darcy's law can be solved as a moving boundary problem under quasi-steady conditions.

The sharp-interface approach is applied to model the infiltration of thermosetting resin into a mold packed with carbon or glass fibers during the manufacture of polymer composite using the liquid composite molding (LCM) process. The woven or stitched fabrics made from carbon or glass fibersused in LCMare often referred to as 'dual-scale' porous media due to the presence of large and small pores. The coexistence and interaction of the 'micro'tow-impregnation flow and the 'macro'inter-tow flowlead to the presence of partial saturation behind the resin front.Adual-scale flow model based on the sharp-front approach is proposed using the mathematically rigorous volume averaging method. Novel multiscale algorithmsbased on fabric unit-cells and hierarchical computational grids are appliedto simulate such an unsaturated flow in the dual-scale fabrics. A good match between numerical predictions and experimentsdemonstrates that the proposed dual-scale modeling can be used successfully to simulate the LCM mold-filling indual-scale fabrics.

Some otherexampleswhere the sharp-front approach can be applied will be presented.They willinclude one on wicking of liquids into polymer or paper based wicks and the other on making of metal-matrixcomposites using the pressure infiltration process.

Participating Project Leader

in Alphabetical Order

Project leader

Michael Baune

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Short CV

Educational background
Dr. rer.nat. Physical and Theoretical Chemistry
Dipl. Chemistry, Bremen University

Current occupation
Bremen Senior Researcher

Research area

- Electrokinetic separation technology
  Dielectrophoretic particle separation
- Recycling & Regeneration
  Upcycling of paperdust
- Electrochemistry Energy conversion
  Material characterization
- MIMENIMA Project
  Investigation of dielectrophoretic effects in porous structures

Project leader

Udo Fritsching

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Short CV

2009	Guest Prof. at Harbin Institute Technology, Harbin, China
2007	Professor at University Bremen
2003	apl. Professor at University Bremen
1999	Habilitation University Bremen, Priv.-Doz., venia legendi in Process Engineering
1990	Research Director Multiphase Flow, Heat and Mass Transfer in the Process Engineering Department of the Institute of Materials Science (IWT), Bremen
1990	Promotion Dr.-Ing. University Bremen
1985 - 1990	Res. Ass. at Process Engineering Dept., University Bremen
1984 - 1985	Res. Ass. at Inst. Practical Mathematics at RWTH Aachen
1983	Diploma Thesis at University of Nevada, Boulder City, USA
1977 - 1984	Studies Mechanical Engineering, RWTH Aachen, Dipl.-Ing.

Reseach area (overview)

Multiphase Flow, Heat and Mass Transfer, Particle Technology, Atomization and Sprays, Thermal Process Technology, Computational Modeling and Simulation

Project leader

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Short CV

since 03/2012	Juniorprofessor für Werkstoffmechanik – Computational Material Modeling University of Bremen
10/2011 – 03/2012	Research Scientist, BIME - Bremer Institute of Mechanical Engineering, University of Bremen
03/2010 – 09/2011	Research Scientist, Department of Scientific Computing, The Florida State University, Tallahassee, FL, USA
09/2006 – 02/2010	Postdoctoral research fellow, Fraunhofer IWM, Freiburg and at IZBS, University of Karlsruhe (TH)
03/2002 – 08/2006	Research assistant, IZBS, University of Karlsruhe (TH), Dr.-Ing. 09/2006

Research area

crystal plasticity, dislocation based modelling of plasticity, deformation texture, forming processes, ductile damage, mechanics of porous materials, statistical materials properties, microstructure – property relations, microstructure evolution, radiation damage

Project leader

Stephen Kroll

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Short CV

Stephen Kroll got his Bachelor and Master Degree in Life Science at the University of Hanover (Germany) and he carried out his Ph.D. thesis aiming at developing a novel hollow fiber micro-bioreactor for cultivation and downstream processing at the Institute of Technical Chemistry, University of Hanover (Germany). In 2008 he joined the Research Training Group “Nonmetallic Porous Structures for Physical-Chemical Functions (PoreNet)” working at the Advanced Ceramics Group, University of Bremen (Germany), as research fellow. In 2011 he became Senior Scientist at the Advanced Ceramics Group, University of Bremen, supervising the working group “Novel Processing and Shaping Routes for Ceramics”. The research activities are mainly focused on porous ceramics for biotechnological and environmental applications.

Research area

- Processing of nanostructured ceramics for biotechnology and environmental applications
- Porous ceramics with adjustable pore sizes and porosities
- Ceramic membranes for separations in liquids (virus and bacteria filter) and gaseous media
- Freeze-casted ceramics
- Ceramic foams/scaffolds for bioengineering applications
- Surface functionalization
- Antimicrobial ceramic surfaces (“antiviral”, antibacterial)

Project leader

Lutz Mädler

Reactive Spraying
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University of Bremen, Germany

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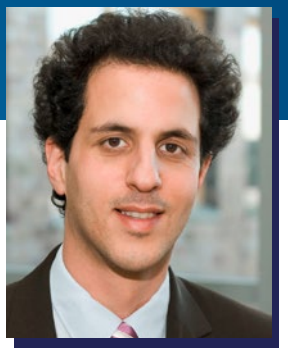
Short CV

Lutz Mädler is a Director of the Process & Chemical Engineering Division of the Foundation Institute of Materials Science (IWT) and full faculty leading the Particle and Process Technology division in the Department of Production Engineering at the University of Bremen. He is also head of the Reactive Spraying group in the Process & Chemical Engineering Division at the IWT.

Research area

Spray processing for particulate materials and functional surfaces, particle science and engineering, particulate systems, reactive and non-reactive spray systems, spray combustion, metal forming, melt atomization, aerosol manufacturing of materials, nanoparticle technology, air pollution, environmental health (“nanotox”).



Chairperson / Project leader

Kurosch Rezwan

Advanced Ceramics
Production Engineering
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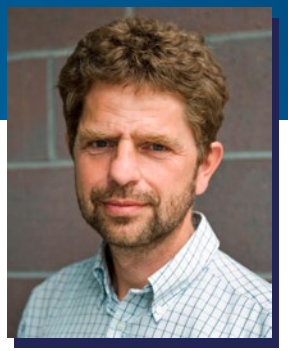
Short CV

Kurosch Rezwan is head of the Advanced Ceramics group and Spokesperson of the research training group MIMENIMA. He obtained his education as a materials scientist at the ETH Zurich and joined after a postdoctoral stay at the Imperial College in London the University of Bremen as a Faculty Member in Production Engineering.

Research area

- Protein interactions with ceramic particles
- Nano- and micro porous scaffolds for bioengineering applications
- Surface functionalized ceramics for biosensor and bioreactor developments
- Antibacterial ceramic surfaces
- Biomimetic ceramic - organic composites
- Advanced ceramic composites



Project leader

Jorg Thöming

Center for Environmental Research
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Short CV

Since 2007 Jorg Thöming is Director of the Centre for Environmental Research and Sustainable Technology (UFT) at University of Bremen, Germany, and Professor of Process Engineering. He received his Diploma (1993) and Ph.D. (1998) degrees from Technical University of Hamburg-Harburg, Germany, both in Process Engineering. From 2000 to 2001 he was DAAD/CAPES-Visiting Professor at Federal University of Rio Grande do Sul, Brazil, where he established process integration. Since 2001 he has been head of the Section of Chemical Engineering - Recovery and Recycling at the UFT, closely cooperating interdisciplinarily with UFT groups from Chemistry, Biology and Social Sciences.

Research area

Green reaction engineering:
- Tailoring of catalytic monoliths: Modelling, NMR imaging, novel systems
- Rarefied gas transport in porous materials

Green separation processes:
- Dielectrophoretic separation and fractionation
- Electrically switchable filters

Green chemistry:
- Structure activity relationships: ionic liquids, nanoparticles
- Electrochemistry and (photo)catalysis
- Upcycling: cellulose-based insulation panels

Project leader

Michaela Wilhelm

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Short CV

Michaela Wilhelm studied chemistry (University of Oldenburg, Germany), where she received her Dipl.-Chem. degree in 1997 and her doctoral degree in 2001, while focusing on inorganic and coordination chemistry. She joined the Advanced Ceramics Group in the department of Production Engineering at the University of Bremen as postdoctoral fellow in 2002, where she later became a senior scientist. Since 2006 her research is additionally integrated in DFG funded research training groups (GRK 1375 PoreNet followed by GRK 1860 MIMENIMA), focusing on porous ceramics and its innovative application. At the same time she acts as coordinator of these programs. She presently works on developing highly porous, multi-functional ceramics and hybrid materials derived from polymers (e.g. polysiloxanes) for application in separation or energy conversion technologies as well as catalysis.

Research area

- Polymer derived ceramics and functional hybrid materials
- Hierarchical structuring of ceramics
- Sol-gel chemistry and surface functionalisation
- Hybrid ceramic catalysts and electrocatalysts
- Highly porous adsorbents with adjusted surface characteristic
- Electron or ion conducting membranes for batteries or fuel cells

Project leader

Thomas Wriedt

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Short CV

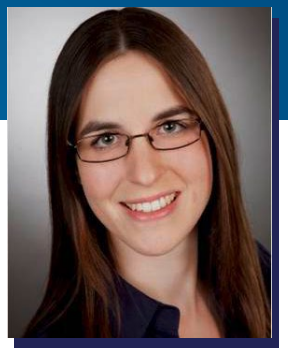
1990 – present	Head of Particle Characterization, Institut für Werkstofftechnik (Materials Engineering), University of Bremen
1987 – 1989	Post Doc Researcher, Institut für Mess-, Regelungs- und Systemtechnik, (Measurement, Control and Systems Engineering) University of Bremen
1986	Dr.- Ing. Degree
1983 – 1986	Scientific Researcher, WE Telekommunikationstechnik (Telecommunication Engineering), University of Bremen
1983	Dipl.- Ing. Degree, Electrical Eng. / Cybernetics, Microwave Engineering, University of Bremen

Research area

- Optical Particle Characterization
- Light scatttering theory
- Surface characterization
- Null-Field Method with Discrete Sources

PhD Students / Postdocs

in Alphabetical Order



PhD student

Julia Bartels

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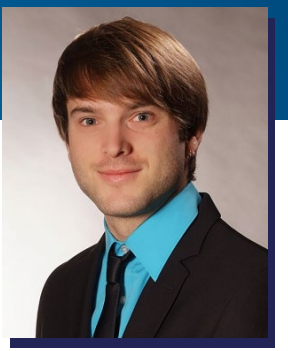
Ceramic capillary membranes with tailored functionalisation and geometry for virus filtration

YSZ powders with different particle sizes (30 nm, 40 nm and 90 nm) are individually and mixed processed by extrusion, dried and finally sintered at 1050 °C for 2 h. The sintered YSZ capillaries are characterised by microstructural analysis including Hg-porosimetry, BET analysis and 3-point bending tests. By increasing the initial YSZ particle size, increased average membrane pore sizes ranging from 24 nm to 146 nm are obtained. Mechanically stable membranes are provided showing high open porosities of ~45 % and ~36 % for capillaries composed of single and mixed YSZ powders, respectively. By increasing the membrane pore size, reduced virus retention capacities in combination with increased water permeate fluxes are achieved. Capillaries made of YSZ-40nm ensure both, log reduction values (LRV) $\geq$ 4 for small model bacteriophages MS2 and PhiX174 and high water permeate fluxes (~30 L/m²hbar), being suitable for sustainable virus filtration as requested by the World Health Organisation (WHO). The capillaries made of YSZ-90nm do not fulfil the virus filter criterion, but can be advantageously used for high flux filtration applications with a water permeate flux of ~460 L/(m²hbar) if an adequate adsorption capacity for viruses by a membrane surface functionalisation with aminosilanes is provided.

Project leader: Kurosch Rezwan, Stephen Kroll



PhD student

Benjamin Besser

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Analysis of gas transport in porous ceramic structures: mesoporous membranes and hierarchical zeolite structures

In the supporting material of asymmetric inorganic membranes gas transport usually occurs in pores >10 nm. Until now, adsorption effects such as surface diffusion are neglected in such pores. I am investigating adsorption effects in porous supporting structures and their influence on the gas transport. For this purpose, the surface of a mesoporous ceramic structure is modified by attaching molecules onto the surface containing different functionalities. Afterwards the influences of the altered surface chemistry is investigated by gas adsorption/desorption and gas permeation measurements.

In separation applications for example in pressure-swing adsorption processes, microporous adsorbents like zeolites or activated carbon are often used. Under these conditions, mass transport limitations play a major role for the efficiency of a process. Hierarchical pore structures provide a possible solution to overcome mass transport limitation to significantly increase the efficiency for adsorption processes. For this reason I am investigating a combination of different processing routes to gain three dimensional, porous structures with hierarchical pore sizes ranging from macro- to microscale.

Project leader: Kurosch Rezwan, Stephen Kroll

Post Doc

Silvia Adriana Collins Abarca

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Development of porous hybrid materials based on silazane and organic monomers for CO_2 adsorption/separation.

Organic-inorganic hybrid ceramics with controlled porosity and large surface area present a great interest due to low cost synthesis and versatile shaping possibilities. It have been applied in different fields as catalysis, adsorption, gas storage. Hybrid ceramics can be obtained by pyrolysis of organic-inorganic polisiloxane based compounds under nitrogen atmosphere. Nevertheless an alternative synthesis can be developed using organic monomers and silazane based compounds to obtain porous hybrid materials by hydrosilylation mechanism reaction assisted by platinum catalyst. This alternative method avoids the normal sol-gel reaction route, reducing some synthesis steps and leading to hybrid porous ceramics with high thermal resistance. Besides the high content of nitrogen atoms in silazane precursors is very useful for CO_2 gas separation since they can induce facilitated transport through the material by reversible formation of carbamates mechanism.

Project leader: Dr. Michaela Wilhelm

PhD student

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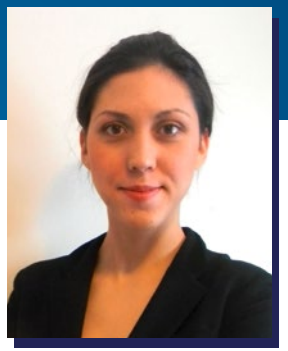
Structural characterization of mesoporous layers using light scattering

In recent years there is a rapid development of inverse light scattering methods to effectively characterize particles. These methods determine the geometric properties of scatterers based on far field scattering patterns.

Measuring the light scattering properties such as extinction spectra or the angular distribution of scattered light of nanoparticles and aggregates on the surface can be used to gauge the accuracy of different light scattering theories in modeling the optical properties of aggregates on a surface and to realize characterization of aggregates on a surface using inverse light scattering methods.

Project leader: Thomas Wriedt, Lutz Mädler



PhD student

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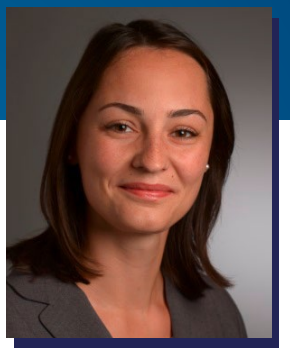
Application of porous ceramics for the handling of cryogenic media in space

The overall aim of the project is to advance the knowledge of the behaviour of cryogenic media in porous ceramic materials. The research effort is on the investigation of the imbibition of a cryogenic liquid into a porous medium (cryo-wicking). In the non-isothermal case, cryo-wicking is accompanied with liquid evaporation, which significantly influences the imbibition. To study the process experimentally, one can measure the mass of the imbibed liquid during the wicking time. Theoretical prediction and CFD simulation of the process are possible with the use of preliminary determined macroscopic parameters, thermo-physical properties of the solid material of the porous structure, thermo-physical properties of the liquid and vapour phases of the cryogenic fluid and environmental conditions.

Project leader: Michael Dreyer



PhD student

Gesa Hollermann

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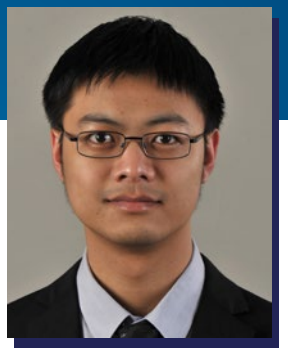
Functionalized porous ceramics for biotechnological application

Enzyme-based technological processes offer a great potential for a resource-efficient, environmentally friendly production and purification of e.g. chemicals or pharmaceuticals. In this project porous oxidic Al_2O_3-SiO_2 ceramics will be fabricated via a novel green chemistry approach based on the ionotropic gelation (IG) of alginate. Featuring hierarchical and adjustable pore sizes from 13 to 184 nm , structure and porosity (up to 90%), high stability in different solutions, high surface area (from 20 m^2/g to 70 m^2/g) as well as high liquid flow permeability. In several project phases, fundamental aspects such as the mutual influence between the material features (e.g. different pore sizes), the surface functionalization with precursors (e.g. amino-silanization), flow condition processes and enzyme-specific properties will be addressed. The rather well characterized enzymes catalase (CAT) and the enzyme glucose oxidase (GOx) will serve as model tandem system, as they perform sequential substrate reactions which are easy to detect. GOx converts ß-D-glucose to D-glucono-δ-lactone and H_2O_2 using molecular oxygen as electron acceptor, whereas CAT decomposes H_2O_2 to water and molecular oxygen.

Project leader: Laura Treccani, Stephen Kroll, Kurosch Rezwan



PhD student

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Nuclear Magnetic Resonance Methods for Characterization of Mass Transport in Porous Materials

Nuclear Magnetic Resonance (NMR) techniques can non-invasively and non-destructively characterize the structure of porous materials and processes in them by relating required information, e.g. porosity, pore size distribution, tortuosity, fluid filling, filtration, etc., and relevant contrasts in NMR techniques, e.g.: proton density, magnetization relaxation times, internal magnetic field, chemical shift, fluid molecular self-diffusion, fluid flow velocity, etc..

The aim of the research project is to improve and develop in situ NMR imaging methods for porous materials with acceptable signal-to-noise ratio and resolution by optimizing NMR pulse sequences, constructing self-built radio-frequency coils, etc..

The applications contain monitoring drying process of fluids in porous materials by utilizing ultrashort echo time imaging methods with high spatial and temporal resolution, calculating tortuosity of porous materials by acquiring diffusion coefficients of fluids in porous materials, studying deep-bed filtration process in porous materials by measuring flow maps of fluids in porous materials, etc..

Project leader: Wolfgang Dreher

PhD student

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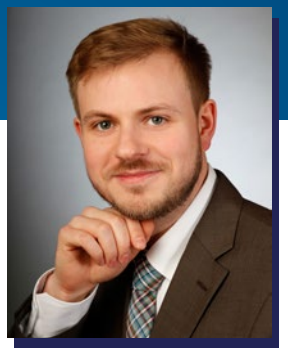
Monolithic Catalysts of Graded Porosity

Monolithic sponges, also known as open-cell foams, have been generating substantial interest as catalyst support in current and recent years. Depending on their porosity and pore count (ppi), they combine large surface areas, low pressure drops, and decent heat and mass transport properties, and are thus well suited as catalyst support for highly endo- and exothermic processes. Three noticeable examples of exothermic processes, which are currently discussed as promising options for long-term storage of excess renewable energy, are the methanation of CO_2 (Power to Gas, PtG), the Fischer-Tropsch process (Power to Liquid, PtL), and the synthesis of methanol (PtL) from green syngas. The performance of these processes, however, depends vitally on the effective removal of heat from the reaction zone to control hot spots that induce thermodynamic limitations, promote undesirable side reactions, and decrease catalyst lifetime. In this project we investigate computationally and experimentally how the structure of monolithic sponges, represented by open porosity and pore count, and further their spatial distribution within the reactor, can be utilized to tune heat transport locally, and thus tailor the axial and radial temperature profiles to balance tolerable hot spots, high yields, and low pressure drops.

Project leader: Jorg Thöming



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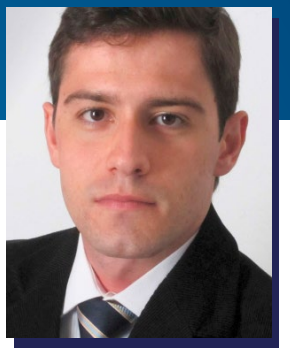
Mechanical Effects of Clusters in Macro-Porous Ceramics

For macro-porous ceramics used in process technology, fracture toughness and structural stability are essential. The mechanical properties of macro-porous ceramics usually show large variations in experiments also at constant porosity. These variations are commonly ascribed to random accumulated pores, so-called clusters. Clusters introduce peak stresses under mechanical load. These peak stresses are critical for crack initiations. There is currently no consistent definition of a cluster. Usual cluster definitions include topological properties and no mechanical interactions between pores. In this project we work on correlations between the tendency of building clusters inside a pore distribution and the failure behavior. Building on this, we aim on a cluster definition based on spatial proximity as well as local stress peaks. These correlations are theoretically analyzed with a suitable number of representative volume elements based on Finite Element Method (FEM). Compression tests with perforated ceramic discs in terms of physical models and with application orientated macro-porous ceramics validate the FEM results. Analyzed in-situ photography and X-Ray tomography images document the local failure behavior during these tests.

Project leader: Thomas Hochrainer



PhD student

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Coacervate-directed calcium carbonate microcapsules for delivery of biomolecules

Microspheres of calcium carbonate loaded with active agents were synthesized using a bio-inspired mineralization technique. Polyacrilic acid (PAA) is used as the additive to modify mineralization, to stabilize amorphous calcium carbonate (ACC) polymorph and to allow the formation of simple coacervates droplets. Simple coacervates are submicron-sized particles that phase separate from the aqueous solution due to electrostatic interaction between calcium ions and the negatively charged polymer. The size of the droplets may be tailored by controlling the polyelectrolyte concentration and the reaction time of complexation. The incorporation of active agents within the coacervates droplets is achieved by dispersing the agents in the aqueous solution prior to phase separation. In order to stop the complexation and to stabilize the loaded-droplets, sodium carbonate is added to the solution leading to mineralization of the coacervate. As the reactions take place under aqueous conditions, at mild pH and room temperature, the process appears to be an effective way to synthesize active-loaded biocompatible ACC microcapsules.

Project leader: Kurosch Rezwan

PhD student

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Formulation and characterization of multiple fluid-fluid dispersions using micro-membranes

Multiple emulsion formulations are widely used e.g. for pharmaceutical purposes for controlled drug release as they allow the encapsulation of active molecules in the aqueous phase. In contrast to a conventional two-component emulsion like water in oil (W-O) or vice versa (O-W), the multiple emulsion system consist of oil-water and water-oil emulsions (W-O-W) simultaneously. The dispersed phase contains itself even smaller dispersed droplets. This type of emulsion is highly unstable, because it consists of two thermodynamically unstable interfaces: the ones of the outer and inner dispersed phases. The aim of this research project is to formulate a stable double emulsion using a novel two stage membrane emulsification process. The development of the setup is assisted by the numerical simulation of a multiphase flow through a porous medium.

Project leader: Udo Fritsching

PhD student

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Chair of Magnetofluiddynamics
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Deep bed filtration in real porous structures – combination of µCT and MRI

Because of a lack of knowledge of the internal processes within deep bed filtration, the filtering efficiency is often described by empirical filtration coefficients. Moreover, the influence of different parameters – such as the porosity or the pore sizes of the filter – on the quality and quantity of deposition is far from being predictable at the current state of research. Additionally, the subject of research in the last decades was the investigation of model systems of filters (e.g. packed beds of glass beads) rather than real filter structures.

Due to these shortcomings, it is the aim of this project to increase the understanding of the deposition processes in real filter structures (e.g. ceramic foams). This will be achieved by applying micro computed X-ray tomography (µCT) as a tool to image the complex inner structure and deposition sites within the filter. Furthermore, a quantitative analysis of the obtained data and thus a detailed understanding of the filtration process itself becomes possible by means of digital image processing.

In addition to the µCT scans, magnetic resonance imaging (MRI) will be applied to image the flow field inside the porous medium, since the flow structure will affect the deposition process considerably.

Project leader: Stefan Odenbach

Postdoc

Prabu Moni

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Synthesis of Multifunctional, Hybrid Ceramics derived from Polysiloxanes for Electrochemical Applications

The commercialization of energy storage and conversion devices needs dramatic improvement in the discovery of cheap and highly effective material with its unique structure to promote its electrochemical performance. Recently polymer derived ceramics being a new class of materials because of their diverse, fascinating topologies and pore size tenability, but they show a poor intrinsic electrical conductivity (<10-10 Scm^{-1} at room temperature). Further, substantial improvements in electrical, thermal, mechanical, and chemical properties of microstructure composites made with a variety of nanoparticles incorporating like carbon nanotubes or graphene in the matrices using covalent and noncovalent methodologies. The goal of this project work is to develop an inexpensive, high surface, porous and catalytically active ceramics using polysiloxanes as polymer backbone with graphene and carbon nanotube as conductive nanofiller for electrochemical applications. Using the advantages from the polysiloxanes and 2D graphene oxide, for the first time we focused to develop a self-assembly of three-dimensional porous chemically modified graphene and carbon nanotube as shell structures for a monolithic polymer derived ceramic core using an emulsion based synthesis strategy. Further, using these materials for potential applications like supercapacitor and zinc-air battery.

Project leader: Michaela Wilhelm, Kurosch Rezwan

PhD student

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Investigation of dielectrophoretic effects in porous structures

This project aims on the continuous separation and recovery of nanoparticles by dielectrophoretic trapping in porous materials. The pore sizes are several orders of magnitude larger than the particle diamter to avoid mechanical filtration.

The porous medium is placed between two electrodes which generate an electric field. The polarization of the filter material causes an electric field disturbance. The resulting inhomogeneous field can be used to polarize and dielectrophoretically move particles towards the pore walls, where they reside until the electric field is turned off. This allows switchable particle trapping with virtually no pressure loss and negligible fouling.

Numerical methods are applied to understand the material and geometry influence on the polarization of the porous medium. Further, the knowledge is used to develop and test several filter structures in a dielectrophoretic filtration process.

Project leader: Michael Baune, Jorg Thöming

PhD student

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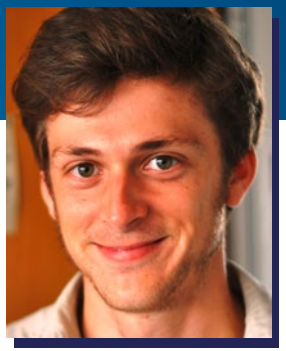
Catalytically active materials prepared from Sol-Gel techniques

The project focuses on Sol-Gel coated monoliths and foams for highly exothermic catalytic gas phase reactions. In comparison to conventional pellet catalysts, a lower pressure drop and less heat/mass transport limitations can be realized by using open porous monolithic supports.

The primary aim is the preparation and testing of catalysts from Sol-Gel-techniques for the CO_2 methanation and Fischer-Tropsch synthesis. In comparison to classical incipient wetness methods, the active phase and the support are directly formed during calcination, leading to benefits such as highly disperse supported particles, special metal-support interactions, and a complex porous network.

Another topic of this project is the investigation of Sol-Gel coatings from on metallic/ceramic monolithic samples and foams. In comparison to the conventional suspension approach, the active phase is formed directly on the support, which offers good adhesive properties.

Project leader: Marcus Bäumer



Postdoc

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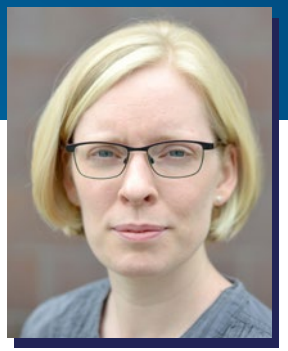
Experimental and theoretical study on multicomponent diffusion gases under rarefied conditions

Multicomponent diffusion of gases in microscale and nanoscale confined geometries is determining the integral behaviour and efficiency of many natural and technical processes. In such small systems the gas is in a state referred to as rarefied where diffusion is the dominating, and hence limiting, transport mechanism. Considerable enhancement on the macroscale in, e.g., membrane gas separation, heterogeneous catalysis, and microelectromechanical systems is only possible when understanding the dependence of gaseous rarefaction on multicomponent diffusion fundamentally. The Maxwell-Stefan equations (MSE) yield reasonable results for bulk multicomponent diffusion but fail for the description of transport under rarefied conditions. Furthermore, in literature all experimental and numerical analysis on multicomponent diffusion confine on uniform ducts as object of examination. This is wondrous since “real” pores are typically tapered and diffusive flux strongly depends on the duct’s cross-sectional area as it was shown in an own earlier work. This project aims for a new, experimentally validated model that allows for the prediction of multicomponent diffusion in uniform and tapered ducts over a wide range of gaseous rarefaction.

Project leader: Jorg Thöming



PhD student

Wiebke Veltzke

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Cellulose-based porous materials - development of a model to determine thermal conductivity

In order to replace non-sustainable insulation materials, e.g., mineral wool, expanded and extruded polystyrene, it is essential to develop new high-performance insulation materials that are sustainable, harmless, and are produced at a reasonable price. For that reason the main working field is the development of a cellulose based insulation material in terms of a paper panel. The main educt of the paper panel is paper dust that appears during the production process of cellulose fibre insulation. The development of such a novel material requires a semi empirical model that allows for the prediction of the thermal conductivity of the paper panel. By means of the model the best solution in terms of process, educts, and additives and mainly thermal conductivity of the paper panel will be identified. In order to achieve this aim the working fields are the characterization of paper dust (main educt) and paper panels (product), model development and implementation, and the construction of an guarded hot plate apparatus to determine the thermal conductivity (target dimension) for the sake of model validation.

Project leader: Michael Baune, Jorg Thöming

PhD student

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Adjustment of Polymer derived ceramics for capillary transport of cryogenic liquid

Ceramics has attracted considerable attention in aerospace applications due to their resistance to thermal shock, corrosive condition, low density, low thermal conductivity and good electronic barrier. Macroporous ceramics show the promise in the delivery of cryogenic propellant. Due to the fact that the elements are designed at room temperature, however, work in cryogenic temperature, it is very important to investigate the thermal properties and mechanical properties under these conditions.

Macroporous monolithic component may be fabricated by freeze casting method use ice as the template, and polysiloxanes as precursors. A hierarchical meso/macroporous SiOC ceramic monolith was obtained. The thermal properties in terms of thermal diffusivity, specific heat capacity and thermal conductivity, and mechanical property in terms of compression strength are investigated at cryogenic temperature. The investigation of these properties of SiOC ceramic materials enables better structure design for low temperature applications.

Project leader: Michaela Wilhelm, Kurosch Rezwan

MIMENIMA Chairperson

Prof.-Dr.-Ing. Kurosch Rezwan

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