



MIMENIMA Summerschool 2022

07.09.-08.09.2022

«Multiphase- and Multicomponent Flows in Material Science»



Multiphase- and Multicomponent Flows in Material Science

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 a diverse cultural and scientific background such as engineering, physics, biology, chemistry, and material sciences work together on tailored novel porous ceramic structures for applications in energy, environment 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 to learn and to adapt for open discussions, to meet possible research partners, and to learn and adapt concepts from other fields.

We wish you an inspiring and exciting meeting!

On behalf of all members of the research training group MIMENIMA

Organisation board

Deepanjalee Dutta
Judith Marie Undine Siebert
Md Nurul Karim
Apostolos Kyrloglou
Adrian Ricke

MIMENIMA Chairperson

Kuroschi Rezwan



07.09.2022	
08:15	Departure from Bremen Central Station
09:30	Arrival and check in inclusive snacks and coffee
10:00 – 10:15	Welcome and Introduction Prof. Rezwan and the organization board
10:15 – 10:45	Flashtalks PhDs
10:45 – 11:00	Coffee break
11:00 – 12:00	Prof. Dr. Mauro Braconi Politecnico MILANO <i>“CFD modeling of single and multi-phase flows with a detailed microkinetic description of the surface reactivity”</i>
12:00 – 13:00	Lunch
13:00 – 14:00	Prof. Dr. Johan Rønby Pedersen Section of Mathematics and Physics Department of Science and Environment Roskilde University <i>“The art of moving a surface”</i>
14:00 - 14:15	Coffee break
14:15 - 15:15	Prof. Dr. Andy Sederman Department of Chemical Engineering and Biotechnology University of Cambridge <i>“MR measurements of single- and two-phase flows in porous structures”</i>
from 15:15	Check into the rooms
16:00 – 17:10	Boat tour on the Zwischenahner Meer with coffee/tea and cake
17:10 – 18:40	Guided Tour “Small Sightseeing Tour with Ammerland Specialties”
19:00 – 20:00	Dinner
20:00 –	Open end

08.09.2022	
07:00 – 09:00	Breakfast and checkout
09:00 – 10:00	Prof. Dr. Judy Lee Chemical and Process Engineering University of Surrey <i>“Nano/Microplastic induced membrane fouling and potential mitigation strategies”</i>
10:00 – 10:15	Coffee break
10:15 – 11:15	Prof. Dr. Patrick Huber Institute for Materials and X-Ray Physics Hamburg University of Technology & Deutsches Elektronen-Synchrotron DESY <i>“Water confined in nanopores: What do we know about it and what is it good for?”</i>
11:15 – 12:15	Moderated open discussion <ul style="list-style-type: none"> • open questions • cooperation/new visions
12:15 – 13:15	Lunch
13:15 – 15:00	Discussion of the project ideas in small groups
15:00 – 15:15	Coffee break
15:15 – 16:15	Presentation of the results
16:15 – 16:30	Closing remarks Prof. Rezwan and the organization committee
17:13	Departure from Bad Zwischenahn Station
18:05	Arrival in Bremen Central Station



Participating Guestspeakers

in alphabetical order

Guestspeaker

Mauro Bracconi

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Short CV

Mauro Bracconi is tenured Assistant Professor of Chemical Engineering at the Laboratory of Catalysis and Catalytic Processes, Politecnico di Milano, Italy. He received his Ph.D. in Chemical Engineering at Politecnico di Milano in 2018. He was visiting scholar at the School of Chemical Engineering & Analytical Science, University of Manchester (UK) from February 2017 to July 2017 and at the Delaware Energy Institute of University of Delaware (USA) in June 2019. He is member of the Early Career Advisory Board of the scientific journal *Chemical Engineering and Processing - Process Intensification*, Elsevier as Editorial Mentee.

Research areas:

- Development of numerical methodologies for the coupling between detailed chemistry (e.g., mean-field and kinetic Monte Carlo) and CFD
- Development of Machine Learning and Artificial Intelligence techniques for advanced catalytic reactor modeling
- Development of methodologies for the multiscale simulations of multi-phase chemical reactor.
- CFD-based investigation of transport properties in innovative catalytic supports

Abstract

CFD modeling of single and multi-phase flows with a detailed microkinetic description of the surface reactivity

Multiscale modelling is widely acknowledged to be a promising route to achieving first-principles-based insights into the reactor and process behavior providing crucial pieces of information to achieve a fundamental understanding of the process under reacting conditions [1]. In particular, Computational Fluid Dynamics (CFD) can describe the flow field and the transport phenomena in three-dimensional complex geometries, while detailed microkinetic modelling and kinetic Monte Carlo simulations have demonstrated unparalleled power in the detailed description of surface reactivity.

The talk will initially discuss the advanced multiscale methodologies capable of describing not only the complex fluid dynamics but also the interactions between species, heat transfer and surface reactivity in heterogeneous reacting flows [2,3]. In particular, the numerical methodologies required to include a detailed description of the surface reactivity in single- and multi-phase systems will be presented with a specific focus on the latter which are of key importance for many industrial processes and to produce clean synthetic fuels from renewables.

Then, some insights will be provided into the methodology used to reduce the intrinsic computational cost of multiscale simulations which usually hinders their application to large-scale industrial systems. Initially, conventional techniques (e.g. in situ tabulation and agglomeration) will be presented followed by an overview of the potential of Machine Learning techniques in facilitating the coupling between first-principles kinetics and detailed numerical simulations [4]

Bibliography

[1] M. Maestri, *Chem. Commun.* 53 (2017) 10244–10254.

[2] D. Micale, et al., *Chemie Ing. Tech.* 94 (2022) 634-561.

[3] M. Bracconi, *Chem. Eng. Res. Des.* 179 (2022) 564–579.

[4] M. Bracconi, M. Maestri, *Chem. Eng. J.* 400 (2020) 125469.

Guestspeaker

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Short CV

Patrick Huber received a diploma and a PhD in physics from Saarland University, Saarbrücken (Germany). After a post-doc in the Physics Department of Harvard University, Cambridge (USA), he did his habilitation in experimental physics at Saarland University (2008). He was a guest scientist at the Max-Planck Institute of Colloids and Interfaces, before he accepted an associate professorship in physics at Pontifical Catholic University of Santiago de Chile in 2011. In 2012 he joined the Institute of Materials Physics and Technology of Hamburg University of Technology (TUHH) as an associate professor. Since 2020 he is the director of the Institute for Materials and X-Ray Physics and head of the research group on High-Resolution X-Ray Analytics of Materials at Deutsches Elektronen-Synchrotron DESY within a cooperative full professorship between TUHH and DESY.

Research areas

- condensed-matter physics
- nanoporous functional materials
- nanofluidics
- X-ray and neutron diffraction

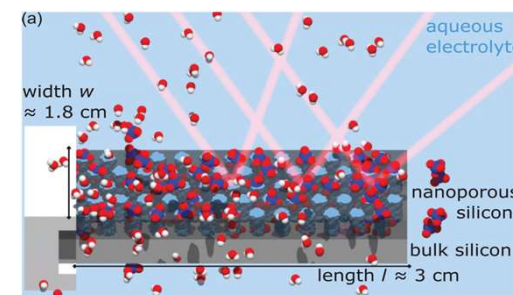


Abstract

Water confined in nanopores: What do we know about it and what is it good for?

Water confined in pores a few nanometers across plays a dominant role in many natural and technological processes ranging from clay swelling, frost heave, and catalysis via colloidal stability and protein folding to transport across artificial nanostructures and bio-membranes. In nanoporous media the geometrical confinement and pore wall-fluid interactions as well as complex pore morphologies may significantly alter water's physico-chemical equilibrium and non-equilibrium properties, causing, for example, the molecular structuring of the fluid, huge negative Laplace pressures in the liquid and changed shear viscosities.

In the first part of my talk I will present opto-fluidic, X-ray and neutron scattering experiments on capillarity-driven transport, self-diffusion dynamics of water and aqueous electrolytes in nanoporous solids [1, 2] as well on the interplay of water's capillarity with the confining solids' elasticity [3, 4]. The observations on the effective, porous-medium scale will be related to the single-nanopore fluid properties [2], also by resorting to computer simulations. In the second part of my talk I will exemplify that exploiting water's peculiar nanofluidics in combination with self-organized porosity in solids offers an entirely novel design space for sustainable, active integrated materials with functional diversity. In particular, I will present porous materials with electrically switchable wettability and hydraulic permeability [5] as well as large electrochemo-mechanical actuation for potential applications in Lab-on-a-Chip fluidics, sensorics, water filtration and energy conversion [5,6,7].



References: [1] Capillary rise of water in hydrophilic nanopores, S. Gruener and T. Hofmann and D. Wallacher and A.V. Kityk, P. Huber, Phys. Rev. E 79, 067301 (2009). [2] Dynamics of water confined in mesopores with variable surface interaction. A. Jani, M. Busch, J.B. Mietner, J. Ollivier, M. Appel, B. Frick, J.M. Zanotti, P. Huber, M. Fröba, D. Morineau. J. Chem. Phys. 154, 094505 (2021). [3] Elastic response of mesoporous silicon to capillary pressures in the pores, G.Y. Gor, L Bertinetti, N. Bernstein, T Hofmann, P. Fratzl, P. Huber, Appl. Phys. Lett. 106, 261901 (2015). [4] Thelen, M.; Bochud, N.; Brinker, M.; Prada, C.; Huber, P. Laser-excited elastic guided waves reveal the complex mechanics of nanoporous silicon. Nat. Comm. 12, 3597 (2021). [5] Switchable imbibition in nanoporous gold, Y. Xue, J. Markmann, H. Duan, J. Weissmüller, P. Huber, Nat. Comm. 5, 4237 (2014). [6] Giant electrochemical actuation in a nanoporous silicon-polypyrrole hybrid material. M. Brinker, G. Dittrich, C. Richert, P. Lakner, T. Krekeler, T.F. Keller, N. Huber, P. Huber. Sci. Adv. 6 eaba1483 (2020). [7] Wafer-scale electroactive nanoporous silicon. M. Brinker and P. Huber. Advanced Materials 34, 2105923 (2022).

Guestspeaker

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Short CV

Dr. Judy Lee received her double degree in B.Eng. (Chemical Engineering) and B.Sc (Physics) in 2002 and her PhD in 2006, both from The University of Melbourne, Australia. In 2007 She was awarded the JSPS Fellowship to spend two years in Japan at the National Institute of Advanced Industrial Science and Technology (AIST). She then returned to the Chemical Engineering Department at the University of Melbourne in 2010 as a postdoc for further two years before being awarded the DECRA (Discovery Early Career Researcher Award) by the Australian Research Council in 2012. In 2015 she took up an academic post at the University of Surrey as a Senior Lecturer and is currently an Associate Professor and Director of Learning and Teaching for the department. Her research group at Surrey is interested in both fundamental work and applied aspects of ultrasound processing and membrane filtration systems, with a particular interest in treatment of emerging pollutants such as pharmaceuticals and nano/microplastics in wastewaters.

Research areas

- membrane filtration, water and wastewater treatment, emerging pollutants
- ultrasound processing, acoustic cavitation, sonoluminescence, sonochemistry

Abstract

Nano/Microplastic induced membrane fouling and potential mitigation strategies

Water and wastewater treatment plants process large volumes of influent liquid and at the same time, also discharges large volume of treated effluent into the environment. With the increase in the presence of microplastics found in these treatment plants[1], there are serious concerns as these treatment plants provide drinking water for people and discharge large volume of effluents either into the environment or used as agriculture irrigation. Most water and wastewater treatment plants contain membrane filtration systems that are susceptible to fouling by particulates such as nano/microplastics[1]. Therefore, to improve operation of treatment plants and separation of nano/microplastic separation using membranes, a better understanding of nano/microplastics fouling on membrane filtration systems is important. This presentation will show using microplastics sourced from a commercial facial scrub (i) how microplastics can easily fragment into nanoplastics[2] (ii) fouling of ultrafiltration membranes by nano/microplastics[3] and (iii) possible mitigation of the fouling via chemical surface treatment of membranes using plasma technology [4] coupled with physical air scouring [5].

References

- [1] M. Enfrin, L.F. Dumée, J. Lee, Nano/microplastics in water and wastewater treatment processes—origin, impact and potential solutions, *Water Res.*, 161 (2019) 621-638.
- [2] M. Enfrin, J. Lee, Y. Gibert, F. Basheer, L. Kong, L.F. Dumée, Release of hazardous nanoplastic contaminants due to microplastics fragmentation under shear stress forces, *J. Hazard. Mater.*, 384 (2020) 121393.
- [3] M. Enfrin, J. Lee, P. Le-Clech, L.F. Dumée, Kinetic and mechanistic aspects of ultrafiltration membrane fouling by nano-and microplastics, *J. Membr. Sci.*, 601 (2020) 117890.
- [4] M. Enfrin, J. Wang, A. Merenda, L.F. Dumée, J. Lee, Mitigation of membrane fouling by nano/microplastics via surface chemistry control, *J. Membr. Sci.*, 633 (2021) 119379.
- [5] M. Enfrin, J. Lee, A.G. Fane, L.F. Dumée, Mitigation of membrane particulate fouling by nano/microplastics via physical cleaning strategies, *Sci. Total Environ.*, 788 (2021) 147689.

Guestspeaker

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Short CV

I am Associate Professor in Mathematics at Department of Science and Environment, Roskilde University. I also run the company, STROMNING APS. My passion is the science of fluid dynamics which is about understanding, predicting and controlling flows in water, air and other liquid or gaseous substances.

I develop mathematical models and numerical algorithms which I implement in computational fluid dynamics (CFD) simulation software – mainly in the open source CFD toolbox, OpenFOAM.

CFD software is used in a wide range of engineering disciplines when designing devices, vehicles and structures where adequate interaction with surrounding or internal fluids is often vital for the success of the end product.

My speciality is numerics for flows involving free surfaces and fluid interfaces. These are important in engineering fields such as coastal, offshore and hydraulic engineering as well as in chemical and process engineering.

Research areas

- Fluid Mechanics
- Computational Fluid Dynamics
- Interfacial Flow Numerics
- Body-Fluid Interaction



Abstract

The art of moving a surface

“What is the best way to numerically represent and advect a complex fluid interface such as the air-water interface of a breaking ocean wave?”

During the past 8 years, I have devoted my research efforts to answering this question. The still ripening fruit of this effort is a new geometric volume of fluid (VoF) methods called IsoAdvector for passive advection of a *sharp* interface across an unstructured finite volume mesh. The method has gained wide use within science and engineering in recent years, partly because of its balance between accuracy and efficiency, and partly because it is made available in the open source CFD software package, OpenFOAM.

In the talk, I will present the basic isoAdvector concept and compare its performance with traditional VoF schemes in simple benchmark tests. I will show examples of its capabilities in high resolution interfacial flow simulations but also touch upon the current limitations and our efforts to overcome these in the quest for ever better interfacial flow numerics. Finally, I hope we can discuss the potential usage of isoAdvector based simulations within the research scope of MIMENIMA.

Guestspeaker

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Short CV

Andy Sederman is a Professor in Magnetic Resonance in Engineering at the University of Cambridge in the Department of Chemical Engineering and Biotechnology where he also gained his PhD in 1998. He works in the Magnetic Resonance Research Centre (MRRRC) where his research focus is on developing magnetic resonance techniques for application to engineering and materials. He has worked extensively in the area of velocity and transport measurement and methods to increase the imaging speed to be able to investigate transient systems, both by fast data acquisition and by utilising innovative reconstruction methods allied to data under-sampling. Areas of application for these methods have focused on single and multi-phase flows, fluid flow in porous media and reaction and hydrodynamics in multiphase reactors. His research is largely funded by the EPSRC and industrial collaborators.

Research areas

- Magnetic resonance technique development for use in chemical engineering and other engineering/physical sciences applications
 - Ultra-fast imaging techniques
 - Sparse sampling and image reconstruction
- Single- and multi-phase flows in porous media
- Operando measurement in catalytic reactors

Abstract

MR measurements of single- and two-phase flows in porous structures

Magnetic resonance as an experimental technique has great potential for investigating applications of fluids in porous media and more generally in chemical engineering. The key attributes which make it the most useful medical diagnostic tomography – non-invasive imaging of opaque objects and sensitivity to a large range of contrast mechanisms – also make it useful for non-medical applications. In addition, the ability to locally measure transport phenomena and chemical composition make it ideally suited to a range of chemical engineering applications.

In this Summerschool talk, we will briefly consider the underlying principles of the measurement methods along with some of the restrictions that they place on the information that can be obtained and how these restrictions may be mitigated against. The talk will then look at a range of case studies which demonstrate how magnetic resonance can be used to probe transport processes in multi-phase systems and what information can be extracted. These will include single- and multi-phase flow in packed beds with examples of both direct flow imaging and measurement of mass transport coefficients, ultra-fast measurements of bubbling systems, transport in rocks and chemical reactions in operando reactors.



Participating Project leaders
in alphabetical order

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Wolfgang Dreher

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Short CV

Wolfgang Dreher is a senior scientist in the in-vivo-MR group of the department of chemistry. He obtained his education as a physicist at the Humboldt University in Berlin and at the Centre of Scientific Instruments of the Academy of Sciences in Berlin, where he completed his PhD in 1990. He joined the University of Bremen in 1991 working at the chair of instrumental analytics of Prof. D. Leibfritz in the department of chemistry, where he completed his habilitation. Since 2009 he is continuing his work on NMR imaging and spectroscopy in the in-vivo-MR group of the department of chemistry.

Research area

- Development of dedicated measurement methods for NMR imaging, localized NMR spectroscopy and NMR spectroscopic imaging
- Characterisation of gas phase reactions by NMR spectroscopic imaging
- Diffusion NMR imaging for temperature measurements and for characterising fluids in porous samples
- Method development and applications of NMR velocimetry
- Chemical Exchange Saturation Transfer NMR imaging for inverse metabolic imaging and pH measurements
- Localised 2D NMR spectroscopy for improved signal separation
- Quantification of NMR data using prior knowledge

Project Leader

Michael Maas

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Short CV

Michael Maas is a senior scientist at the Advanced Ceramics group at the University of Bremen. He studied chemistry at TU Dortmund and completed his PhD in Physical Chemistry in 2008, also at TU Dortmund. He then spent two years as a postdoc at Stanford University after which he joined the University of Bremen where he habilitated in 2018.

Research area

- Colloidal assembly of multifunctional nanostructures
- Organic/inorganic Hybrid-Materials
- 3d Printing
- Nanofibers
- Thin Films
- Microcapsules
- Bio-Nano and Bio-Material Interactions

Project Leader

Lutz Mädler

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Short CV

Lutz Mädler studied Physics, Technical Physics and Chemical Engineering in Zwickau and Freiberg, Germany and holds both degrees. He obtained a Habilitation from ETH Zürich where he stayed for 5 years before taking a lectureship and research position at University of California Los Angeles for several years. He is now a Professor in Production Engineering faculty at the University of Bremen, Germany. He also serves as one of the Directors of the Leibniz-Institute for Materials Science.

Research area

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

Chairperson/ Project Leader

Kurosch Rezwan

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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

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Short CV

Jorg Thöming received his PhD from Technical University Hamburg (Germany) in 1998. Following a position as visiting professor at the Chemical Engineering Department at the Federal University of Rio Grande do Sul (Brazil), he joined the University of Bremen as Professor of Chemical Process Engineering in 2001.

Research area

- Recovery processes with focus on novel separation processes
- Chemical energy storage
- Mass and heat transport in catalysts, *operando* analysis on reactor scale
- Electrochemical processes

Project Leader

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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 (PDC) 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 (microbial) fuel cells
- Adapting freeze casting, tape casting phase inversion and 3D printing to polysiloxanes
- PDC monoliths and screens for capillary transport of liquids

PhD Students in alphabetical order

PhD Student

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Short CV

Pedro Braun studied Materials Engineering at the Federal University of Santa Catarina (BR), where he graduated in 2018 with a Bachelor degree/diploma. In 2019, he started his collaboration in the research training group MIMENIMA as a qualifying student in the Advanced Ceramics Group and later as a research associate.

MIMENIMA Project: Polymer-derived ceramics with graded structures for phase separation and catalysis

Porous ceramics are critical for applications such as phase separation in liquid acquisition devices (LAD) and anodes for microbial fuel cells (MFC). Polymer-derived ceramics (PDC) are materials that can be processed at lower temperatures compared to conventional ceramics and can be formed by polymer-shaping techniques such as freeze-casting. Freeze casting is a method that allows a wide range of pore morphologies, pore size distributions, pore directions and open porosities to be tailored by tuning the freezing medium/plate, freezing process and solid loading. Modifying one of these steps allows to tune the resulting pore morphology and thus mass transfer and mechanical properties accordingly. Furthermore, combining the freeze-casting process with direct ink writing (DIW) of PDC-based inks promises the possibility of optimizing porous 3D lattice structures. The aim of this PhD project is to develop ceramics from polymeric organosilicon precursors produced by freeze-casting and/or direct-ink writing and to optimize them for phase separation or as electrode materials in MFCs

Project leader: Michaela Wilhelm

PhD Student

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Short CV

Stefan Endres is currently a doctoral student in the Faculty of Production Engineering at the University of Bremen in the MIMENIMA research group advised by Professor Lutz Mädler. He obtained B.Eng. (Hons.) (2016) and M.Eng. (2018) degrees in Chemical Engineering at the University of Pretoria. His master's thesis was on the topic of global optimisation of free energy surfaces while working at the Institute of Applied Materials in Pretoria, South Africa. He is currently working at the Leibniz-Institute for Materials Engineering in Bremen on the topic of multiphase simulation of mesoporous nanoparticle films.

MIMENIMA Project: Simulation of structural changes of mesoporous films and layers during liquid infiltration and drying

The overarching goal of the project is to model and simulate the structural changes of mesoporous films during the process of fluid imbibition and drying. Mesoporous films built up from hierarchical assemblies of ceramic nanoparticles, referred to as "primary particles" form complex structures of aggregates (percolated, chemical bonded or "sintered" assemblies of particles) and agglomerates (physically bonded primary particles and aggregates).

Project leader: Lutz Mädler

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Short CV

Tongwei Guo studied chemistry at University Duisburg-Essen, where she graduated with a master's degree in science in 2018. She joined the MIMENIMA research group in 2019.

MIMENIMA Project: Plasmonic Porous Ceramics

Design and fabrication of Plasmonic porous ceramics aim to combine the excellent optical properties of plasmonic materials with the advantages of ceramics. As a result, the plasmonic porous ceramics could be applied for highly sensitive, highly selective and rapid detection of molecules under high temperature/pressure conditions.

Project leader: Michael Maas

PhD Student

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Short CV

Md Nurul Karim studied Electrical & Electronics Engineering at the Bangladesh University of Engineering and Technology. After finishing his bachelor's degree in 2013 he worked for some years as an automation and computer vision engineer. Md Nurul Karim obtained his master's degree in control, microsystem and microelectronics from the Universität Bremen in 2019. He joined the MIMENIMA research group in the same year.

MIMENIMA Project: Computer analysis of complex porous ceramic structures.

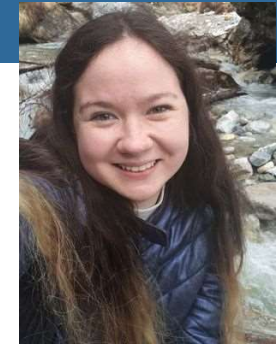
In today's fast-paced industries, there is an urgent need for a rapid production of new materials which satisfy current and future needs. Using techniques that include mathematical modeling and optimization, machine learning and data analytic has shown great potential in reducing the complexity of rationally design new materials and their characterization. This project aims at using material informatics for reducing the time and effort required to characterize complex ceramics structures using micro CT analysis and data-driven machine learning modeling. The benefit of this project will be less experimentation and processing work needed for processing complex ceramic materials for specific applications. This study includes the preparation of datasets, results from numerical simulations, lab experiments, verification of the model from experiments, and 3D convolutional neural network based deep learning on 3D images.

Project leader: Kurosch Rezwan

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Short CV

Mariia Kepper studied at Friedrich Shiller University of Jena and wrote her Master's Thesis at Fraunhofer IOF under the supervision of Dr. Fabian Steinlechner, devoted to an investigation of packaging of the core components of an entangled photon source with laser-based soldering technique (which has a potential to be used in the harsh environmental conditions). Since then she became inspired by material science and now is involved into chemical engineering tasks of water purification (i.e. micro plastics contaminations). She participates in the program of the University of Bremen devoted to a study of Micro-, meso- and macroporous nonmetallic Materials: Fundamentals and Applications (MIMENIMA).

MIMENIMA Project: Investigation of dielectrophoretic effects in porous structures
A contamination of water with micro and submicron particles is a global concern of our days. The recovery of these particles (from now on referred to as target particles) in the micro and submicron range is facing a challenge in the search for a reliable and inexpensive technology that is capable of separating these TP from the liquid. In a series of previous publications, it was shown that dielectrophoresis (DEP) can be a well-suited choice for this task, especially, if the selective separation is required. DEP itself is a particle manipulation technique which requires no target particle charge or labeling. It is caused by the net force on an induced dipole in the target particle in an inhomogeneous electric field. The efficiency a DEP separation technique is directly depending on, among other parameters, electric field gradient (comes from scattering of the field at material boundaries), particle and medium dielectric properties and a size of the target particle. Building on the theoretical results of the previous generations of MIMENIMA, our interest concentrates on the problem of scattering of the electric fields at the material boundaries and on investigating the potential ways to enhance the filtering efficiency.

Project leader: Michael Baune

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Kevin Kuhlmann

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Short CV

Kevin Kuhlmann studied Biomimetics at the University of Applied Sciences in Bremen. During the Bachelor program he did a four months research internship at the Columbia University in the City of New York (New York City, USA) in the field of biomedical engineering. After finishing his bachelor's degree in 2016, he continued studying production engineering at the University of Bremen. Until his graduation in 2019 he did several projects in the field of numerical fluid dynamics, including his master's thesis at the Center of Applied Space Technology and Microgravity in Bremen. He joined the MIMENIMA research group in 2019.

MIMENIMA Project: Mass transport in graded monolithic catalyst supports for strong exothermal gas phase (and multiphase) reactions
Catalytic reactors play an important role in the wide area of process engineering. They are key for the production of chemicals but also for the storage of energy, which is of utmost importance relating to the transformation of the energy system towards 100% renewable energy. Although catalytic reactors have been used for many decades, the exact processes within the reactor are still to be understood. This project aims at simulating both mass and heat transport as well as the reactions itself within the reactor and validate these simulations with experiments using the NMR technique. The results will lead to a better understanding of the processes within the reactor, since the simulations allow a precise insight into the whole system.

Project leader: Jorg Thöming

PhD Student

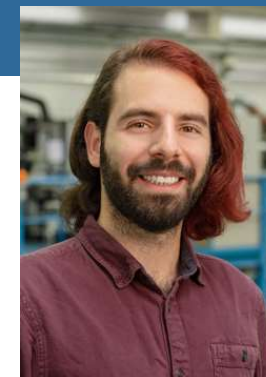
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Short CV

Apostolos Kyrloglou studied Chemical & Process Engineering at the University of Surrey before obtaining a Master's on Advanced Materials & Processes from the FAU Erlangen. He then directly joined the MIMENIMA research group in 2019.

MIMENIMA Project: Transport, Separation, and Mixing of Complex Multiphase Fluids in Pores and Porous Membranes with Varying Surface Activities

In recent years the role of emulsions has been of increasing importance in the food and pharmaceuticals industries. Customer demand for higher product quality together with adherence to increasingly strict government regulation has made studying the emulsification process and its influencing parameters as relevant as ever.

Emulsification is, in its nature, a dynamic and highly transient environment of fluid motion in extremely confined spaces. As such the stresses exerted between the fluids and the membrane walls as well as between the fluids themselves at their interface can rise to significant orders of magnitude.

The aim of the project is to study different fluids and process parameters as to their influence on droplet formation, break-up, and transport in such porous membranes and draw a comparison between experiments and simulated results.

Project leader: Udo Fritsching

PhD Student

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Short CV

Adrian Ricke studied physics at the University of Osnabrück and during this time he published various papers in the field of EPR (electron paramagnetic resonance) spectroscopy. He graduated with a master's degree in 2019 and later joined the MIMENIMA research group in the same year.

MIMENIMA Project: NMR methods for the characterisation of mass transport and reaction processes in porous materials

This project aims at developing and applying novel or improved NMR methods for characterizing mass transport (flow, diffusion, dispersion) and catalytic reactions (concentration of reactants and products, temperature distribution) of fluids (gas, liquid) in porous materials.

Project leader: Wolfgang Dreher

PhD Student

Judith Marie Undine Siebert

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Short CV

Judith Marie Undine Siebert studied General Engineering Science with Major Medical Engineering (B.Sc. 2016) as well as Product Development, Materials and Production (M.Sc. 2018) both at Hamburg University of Technology. After a research stay in the field of Material Science in Brazil (Universidade Federal de Santa Catarina) and a first experience in Industry at Airbus, she joined the MIMENIMA research group in 2019.

MIMENIMA Project: Detection of colloid motion in deep bed filtration processes by means of Fast-X-Ray-Tomography
Deep bed filtration is a complex process, driven by manifold interacting mechanisms on various scale levels. With established 3D imaging techniques such as X-ray μ -tomography and NMR flow measurements it is possible to measure the filter loading at different times and the three-dimensional flow field. The aim of this project is the development of methods, which allow the tracking of colloid motion on the one hand and colloid deposition on the other hand. For this purpose, fast-tomography measurements will be carried out for an adapted model-filtration experiment. The motion of single particles has to be tracked individually and will be visualized by traces in the tomographic data. Particle deposition sites and their spatial position may be identified as partial volumes. The advantages of μ CT and NMR flow measurements can thereby be combined in one method. The combination of filtration experiments, NMR flow measurements and numerical simulations of multiphase flow in high complex geometrical structures allows the scaling of microscopic colloid retention and deposition mechanisms to macroscopic models.

Project leader: Stefan Odenbach



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MIMENIMA Summerschool Bad Zwischenahn,
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