Universität Bremen

MAPEX Center
for Materials and Processes

PROGRAMME

15th MAPEX Early Career Researcher Workshop

BUILDING BRIDGES
across the borders defined by the faculties and institutes

8th June 2023
AIB building (Hochschulring 40)

MAPEX Bremen

Programme overview

8:30	**Registration and poster mounting**
Session 1	
9:00	**Welcome note and introduction** Dr. Hanna Lührs, Dr. Enis Bicer *MAPEX Center for Materials and Processes*
9:15	**The crystal structure of really small crystals using electron crystallography** Dr. Paul Benjamin Klar *Department of Geosciences, University of Bremen*
9:45	**Advancing openness in scholarly communication: Open Access Publishing at University Bremen** Dörte Kanis *Projekt manager Green OA/Self-Archiving at University Bremen/SuUB Bremen*
10:00	**Flashlight presentations (part 1)**
10:30	**Poster session (part 1) / Coffee break**
Session 2	
11:15	**Modeling Metal Oxides** Dr.-Ing. Ingmar Bösing *Group Leader Chemical Process Engineering Group (CVT), University of Bremen*
11:45	**The Data Science Center at the University of Bremen - Interdisciplinary hub, services and support for data-intensive research** Dr. Sandra Zänkert / Dr. Lena Steinmann *Data Science Center*
12:15	**Flashlight presentations (part 2)**
12:45	**Poster session (part 2) / Lunch break**

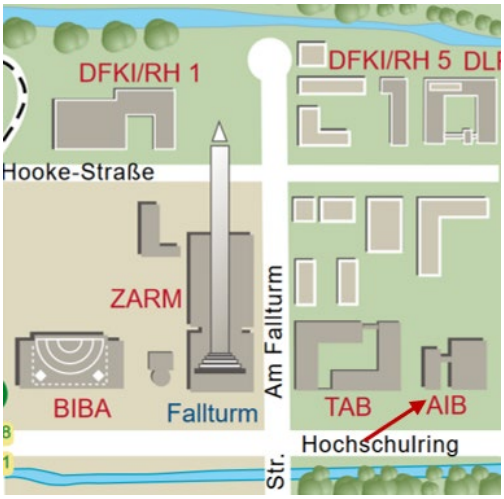
Session 3	
13:45	**Additive manufacturing of iron-based shape memory alloys** Dr.-Ing. Anastasiya Tönjes *Leibniz-IWT, University of Bremen*
14:15	**Adaptive Finite Elements meet Production Engineering** Prof. Dr. Andreas Rademacher *Center for Industrial Mathematics (ZeTeM), Faculty 3 - Mathematics and Computer Science, University of Bremen*
14:45	**Linking photonic and thermal material properties of semiconductor nanostructures** Prof. Dr. Gordon Callsen *Institute of Solid State Physics, University of Bremen*
15:15	**Discussion on academic career path** Prof. Dr. Andreas Rademacher / Prof. Dr. Gordon Callsen
15:45	**General discussion / Coffee break**
16:00	**End of workshop**
17:00	**Get together / social event** Minigolf and dinner *"Zum Platzhirsch" (Kuhgrabenweg 30, 28359 Bremen)*

Venue

AIB building

Hochschulring 40

First floor



Session 1

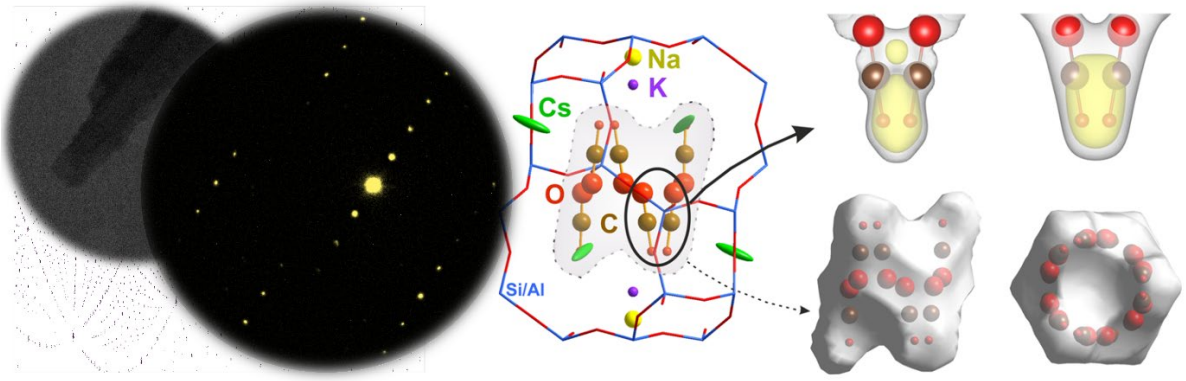
09:00 **Welcome note and introduction**

Dr. Hanna Lührs, Dr. Enis Bicer
MAPEX Center for Materials and Processes

09:15 **The crystal structure of really small crystals using electron crystallography**

Dr. Paul Benjamin Klar
Department of Geosciences, University of Bremen

The understanding, optimisation and modelling of any material is based on the knowledge of the crystal structure. It is therefore no surprise that the most cited paper of the 21st century describes a tool to solve and refine crystal structures from X-ray, neutron, and electron diffraction experiments (Sheldrick, 2008). Though X-ray crystallography is the *de facto* standard for structure analysis, electron diffraction (ED) is catching up, especially if the sample under investigation consists of submicrometric to nanosized crystals. Developments of the last decades and ongoing improvements have made 3D ED a valuable tool for essentially all classes of crystalline materials, including metal-organic frameworks, zeolites, minerals, pharmaceutical compounds, and proteins. This presentation gives an overview on the applications of 3D ED with a focus on selected results on organic compounds, minerals, and zeolites.



09:45	**Advancing openness in scholarly communication: Open Access Publishing at University Bremen**

Dörte Kanis
Projekt manager Green OA/Self-Archiving
University Bremen/SuUB Bremen

This 15 min lecture explores the possibilities of publishing open access articles, specifically focusing on three prominent models: Gold Open Access, Green Open Access, and Hybrid Open Access.

Gold Open Access entails publishing articles in fully open access journals, ensuring immediate and unrestricted access to research. Green Open Access involves self-archiving or depositing articles in repositories or institutional platforms, making them freely accessible after an embargo period. Hybrid Open Access combines subscription-based publishing with open access, allowing authors to make individual articles openly available within otherwise subscription journals.

The lecture highlights the benefits and challenges of each model. It emphasizes the importance of open access publishing in accelerating the dissemination of research, facilitating collaboration, and maximizing the societal impact of scholarly outputs.

By understanding the options available through Gold, Green and Hybrid Open Access, researchers can make informed decisions about choosing the most appropriate publication pathway for their work, based on their goals and resources, and then know when to take the steps along the way.

Staats- und Universitätsbibliothek Bremen

OPEN ACCESS

10:00 Flashlight presenations (part 1)

P01 Molecular dynamics (MD) simulations of a trimeric chaperone complex for the disaggregation of Huntingtin

Annika Niemann
Faculty 04 - Production Engineering, University of Bremen

Classical molecular dynamics (MD) simulations were performed to unravel the molecular mechanisms behind the first steps of a chaperone cycle proven to suppress the aggregation of mutated Huntingtin (HTT) proteins and subsequently the manifestation of Huntington‘s disease (HD). To gain insight into the process, dimeric chaperone-ligand complexes consisting of DNAJB1, Hsc70 and a mutated HTT peptide were formed, and the conformations and interactions observed during simulation were analysed.

P02 Alternative Cathode Fabrication for Lithium-Ion Batteries Using Flame Spray Pyrolysis

Tim Klotz
Faculty 04 - Production Engineering, University of Bremen

The Lithium-Ion Battery (LIB) is known for its high energy density, efficiency and long life. Flame Spray Pyrolysis (FSP) is a promising technique that addresses production process challenges such as scalability, process control, material diversity and cost. Using FSP it is possible to produce ultrafine, phase-pure and crystalline battery electrode active materials at nanoparticle scales. The spinel $LiMn_2O_4$ is a promising cathode material for rechargeable LIBs due to its excellent properties.

P03 Ultrasonic welding of thermoplastic composites: Explicit dynamic analysis of heating mechanisms

Jan Yorrick Dietrich
Faculty 04 - Production Engineering, FIBRE

Ultrasonic welding is a promising technology to enable fast joining of thermoplastic composites while remaining the structural integrity of fibers. This work provides a modeling approach of the heating mechanisms. To cover thermomechanical dissipation, high speed footage of the interaction between the sonotrode and the adherends was analyzed via digital image correlation to be used as a boundary condition in Abaqus/Explicit Fully coupled temperature-displacement simulations.

P04 **Application of Dynamic Electrochemical Impedance Spectroscopy for the study of interfaces in energy storage devices**

Federico Scarpioni
Faculty 04 - Production Engineering, Fraunhofer IFAM

EIS is a powerful technique able to reveal and separate processes of an interface in a non-destructive way. There are high requirements for the collection of impedance spectra on a broad range of frequencies. To overcome them a technique has been developed called dynamic electrochemical impedance spectroscopy (DEIS). DEIS measurements have been used to characterize the interface in different energy storage devices such as supercapacitors, sodium-ion batteries and lithium-ion batteries.

P05 **Bark as a natural model for the flame protection of 3D-printed composite materials**

Thiemo Benthien
Faculty 04 - Production Engineering, University of Bremen

When trees are exposed to fire, the bark protects them for a certain period of time as a natural flame retardant. Density and composition play a role, in addition to other parameters. This study investigated whether an abstracted bark, in the form of a test specimen with a lower density, has more suitable burning properties than a test specimen with a higher density. It also investigated whether the addition of wood flour improves the fire resistance.

Poster session part 1 / coffee break
10: 30 – 11:15

Session 2

11:15 Modeling Metal Oxides

Dr.-Ing. Ingmar Bösing
Group Leader Chemical Process Engineering Group (CVT), University of Bremen

Metal oxides play an important role in catalysis, electronic devices, semiconductor technologies, and corrosion science. Understanding oxide film growth, reduction, and general properties can help in developing specific catalysts, such as those used in water electrolysis, predicting and preventing corrosion processes, and improving electrochemical steel production from iron ores.

Our working group has developed a model to describe the growth of metal oxides, starting from the formation of the first layer, through continuous oxide film growth, until the breakdown of oxide films and failure of the protective layer. The model provides insights into general processes at the metal/film and film/surrounding interfaces, as well as into transport and reaction processes and potential distributions within the oxide film. In addition to applying the model to understand corrosion processes, we are currently collaborating with Robert Bosch GmbH to use the model for corrosion prediction. We are also working on extending the model for electrochemical iron oxide reduction to enhance environmentally friendly steel production.

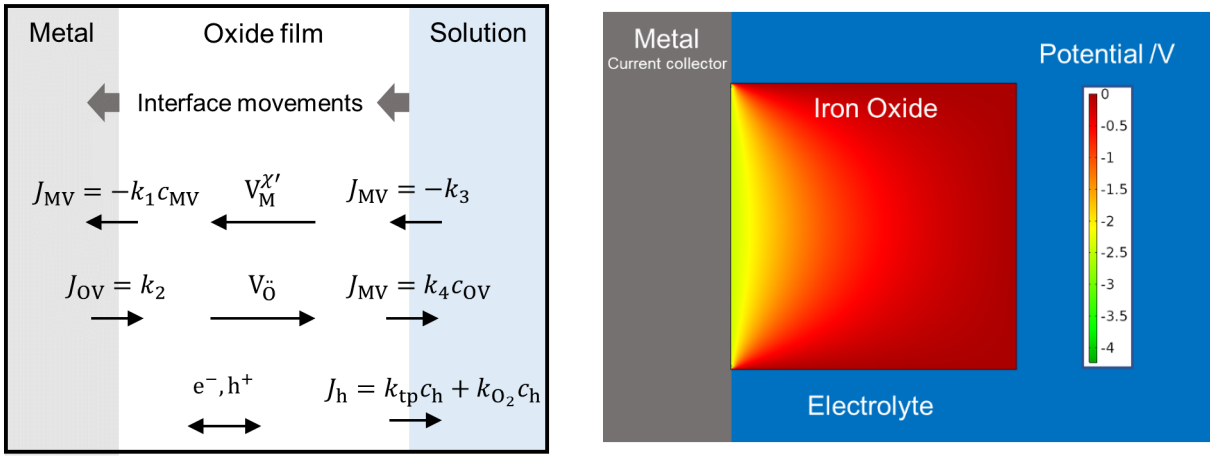
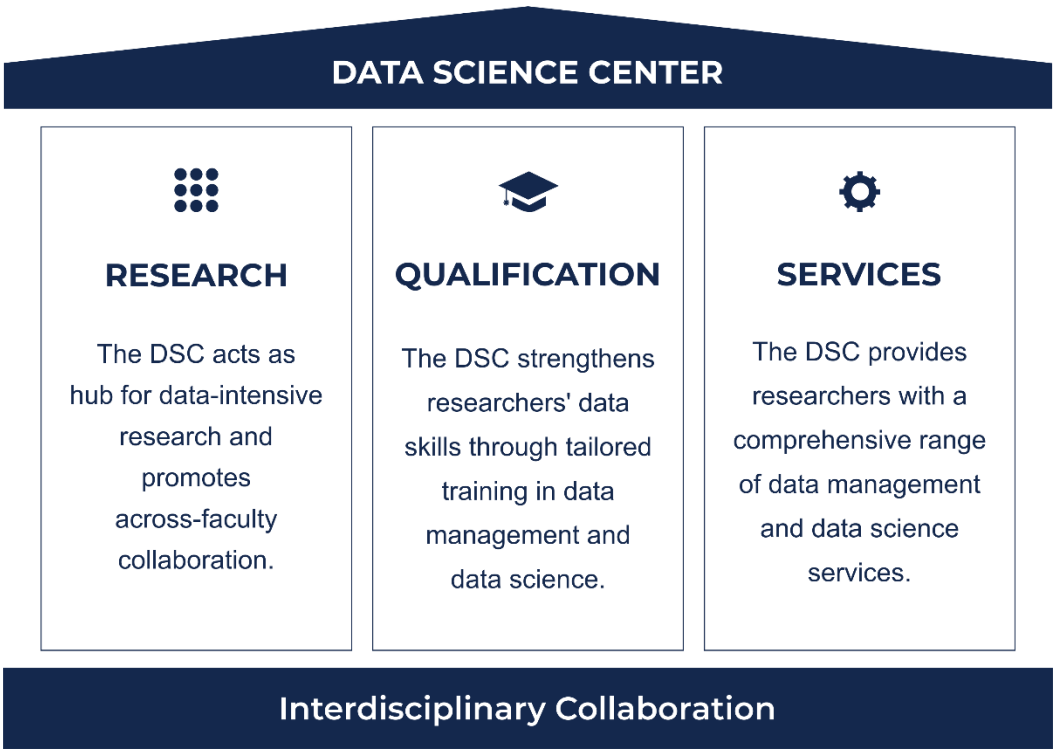


Figure 1: Modeling of metal oxides a) Schematic view of transport processes and boundary conditions; b) Potential distribution inside iron oxide pellets at the initial stage of oxide pellet reduction.

11:45 **The Data Science Center at the University of Bremen - Interdisciplinary hub, services and support for data-intensive research**

Dr. Sandra Zänkert / Dr. Lena Steinmann
Data Science Center

As a result of digitalization, huge amounts of heterogeneous data are produced across all scientific fields, economic sectors, and even in our daily lives, which can no longer be handled with conventional analytics tools. The emerging field of data science provides the methods and technologies to harness the full potential of big data and transform it into knowledge. Hence, data science is considered as key discipline for the modern digital society. However, in order to be able to apply data science methods such as machine learning, the data must be FAIR (**F**indable, **A**ccessible, **I**nteroperable, **R**e-usable). Accordingly, sustainable data stewardship is a basic prerequisite for data science.
During our talk, we will address why the two topics are inseparable and of fundamental importance for science and for early-career researchers. Moreover, we will introduce the services of the Data Science Center (www.dsc-ub.de) at the University of Bremen that researchers can use to improve their data-intensive research and unlock the full potential of their data. These include computational resources (e.g., GPU servers), data literacy training, financial support (DSC Seed Grant), consultation on the implementation of data science methods (e.g., machine learning), and extensive data management services offered by data stewards.



12:15 **Flashlight presenations (part 2)**

P06 **New solid-state electrolyte based on 2-adamantanone for sodium all-solid-state batteries**

Joshua Budde
Fraunhofer IFAM

In this poster a new plastic crystal electrolyte system based on sodium salts and 2-adamantanone, which belongs to the material class of plastic crystals, is presented. Here, the chemical, physical and electrochemical behavior in dependence on the sodium salt concentration is investigated. The results reveal that the solid phase is stable over a wider temperature range compared to the commonly used succinonitrile.

P07 **The role of the membrane in the hen's egg as a model for increasing the toughness of engineered brittle materials**

T. Raphael Woida
Faculty 04 - Production Engineering, University of Bremen

In contrast to a ceramic plate the fragments of a hen's egg stay connected after fracture. This behaviour was investigated as a potential model for engineered brittle materials. Since the eggshell is connected to the biopolymer membrane the influence of this membrane and artificial membranes made from polymers were tested. Compression testing and fracture pattern analysis were used to evaluate the influence of both. A significant influence of the natural and artificial membranes was found.

P08 **Coffee silver skin phytoextracts Characterization and Formulation of Sustainable Disinfectant**

James Ziemah
Constructor University Bremen _ Life sciences and Chemistry

Aerosol hygiene solutions were prepared using coffee silver skin phytoextract and tested in a controlled 20 m3 room which effectively reduced airborne bacterial, yeast and mold. Environmental conditions, temperature and humidity were monitored using data loga. Through chemical characterization using LC-ESI-QTOF-MS, chlorogenic acids were identified as potential active agents in the phytoextract.

P09 Fuzzy Segmentation of Pores in CT of Ti64 AM parts

Pascal Dinglinger
Faculty 04 - Production Engineering, University of Bremen

X-Ray Computed Tomography (CT) for metallic Additive Manufacturing (AM) parts presents challenges in binary labeling due to indistinct boundaries and labeling inconsistencies. I propose using fuzzy segmentation algorithms to generate probability maps that represent defect labels with greater precision. These probability maps can serve as a robust baseline for machine learning methods, particularly in high quality label-dependent applications such as Process Monitoring for Defect Detection in AM.

P10 Isolation and Structure Elucidation of Secondary Metabolites from Tricholoma sulphureum

Lena Ehlers
Faculty 04 - Production Engineering, University of Bremen

Fungi such as Tricholoma sulphureum produce characteristic secondary metabolites as chemical signals or defence mechanisms. These might act as a basis for pharmaceuticals or pesticides and were isolated using high performance liquid chromatography. The molecular structures of the four so called Tricholomol A-D were determined using mass, structural formula, and fragmentation from electrospray-ionisation tandem mass spectrometry together with 1D and 2D spectra from nuclear magnetic resonance.

Poster session part 2 / lunch break
12:45 – 13:45

Session 3

13:45 Additive manufacturing of iron-based shape memory alloys

Dr.-Ing. Anastasiya Tönjes
Leibniz-IWT, University of Bremen

Shape memory alloys (SMAs) are functional materials with unique properties of shape memory effect and pseudo-elasticity. These effects are based on a fully reversible, diffusionless martensite-austenite phase transformation.

The shape memory effect has been studied and detected for multiple alloys, with nickel-titanium being the most researched system. NiTi alloys show a large shape memory effect but exhibit the disadvantages of high production costs and difficult processability. Responding to the demand for more economical materials, research has been conducted on Fe-based shape memory alloys. In addition to low material costs, these are characterised by significantly simplified machinability and weldability. Further research is necessary to improve the shape memory effect of iron-based shape memory alloys. One method to enhance the shape memory effect is modifying the alloy composition.

Iron-based SMAs have mainly been produced conventionally. The research on manufacturing SMAs with additive manufacturing has been limited. In my talk, it will be shown by the example of two FeMnSi-based alloys with different Mn contents that the iron-based shape memory alloys can be successfully processed with laser powder bed fusion. Furthermore, it will be demonstrated how small changes in the Mn content affect the optimal process parameters and shape memory effect.

14:15 Adaptive Finite Elements meet Production Engineering

Prof. Dr. Andreas Rademacher
Center for Industrial Mathematics (ZeTeM),
Faculty 3 - Mathematics and Computer Science,
University of Bremen

The Finite Element Method (FEM) is a commonly used approach for the numerical solution of partial differential equations (PDE). We focus in particular on adaptive Finite Elements. Here, the simulation is optimally adapted to the underlying problem based on so called a posteriori error estimators, which indicate the distribution of the discretization error. Machining processes such as drilling, grinding, or milling, but also forming processes can be modelled by PDEs. In this talk, we discuss the modelling of certain processes and the corresponding adaptive FE simulation. First, we consider a grinding process with special attention to the interaction between the grinding process and the structure of the grinding machine. The dynamics of this interaction is a major challenge. This topic was addressed in the author's dissertation. Next we come to a deep hole drilling process with minimum quantity lubrication. Here, the focus is on the thermal effects and the changing workpiece. Using an example from sheet-bulk-metal-forming, so called model adaptive techniques are discussed, in which the mathematical model is adaptively changed. Finally, we present some results on optimal control and parameter identification using the example of a rolling process and a bolt-nut connection. Parts of this work are included in the author's habilitation thesis or are ongoing research.

14:45 Linking photonic and thermal material properties of semiconductor nanostructures

Prof. Dr. Gordon Callsen
Institute of Solid State Physics, University of Bremen

During the last decades, significant research efforts were devoted to the optical properties of semiconductor nanostructures, enabling fascinating insight into the underlying physics, which already entailed numerous real-world devices like light-emitting diodes and laser diodes. However, the high level of sophistication reached for such photonic devices is contrasted by scarce knowledge about related thermal phenomena, ultimately limiting device functionality, efficiency, and longevity. Thus, it shall be the aim to fill this void by bridging the fields of nano-photonics and nano-thermometry based on a hybrid spectroscopic approach that enables simultaneous studies of optical and thermal material properties. Therefore, the envisioned research has to answer the fundamental and in physics often reoccurring question: How can we define and measure temperature on the nanoscale?

Ultimately, the employed hybrid spectroscopy will either probe the temperature of the phonon or charge carrier bath along with the optical material properties, which jointly provide access to the weighting in between the different contributions to thermal transport given by charge carriers, excitons, and thermal THz phonons. Clearly, such spectroscopy needs to spatially and temporally resolve the temperature field across nanostructures, which can be achieved by a setup recently developed at the University of Bremen. This optical setup will prove pivotal to an understanding of the transport of thermal phonons and charge carriers, which also requests a thorough understanding of the related couplings. Eventually, this understanding will even pave the way to novel thermal designs and circuits.

Consequently, it is the aim to obtain an interlinked understanding of photonic and thermal material properties, which will in this talk be exemplified by the discussion of some first experimental results. Future mutual optimizations based on this understanding shall not only benefit classical optical, electrical, and thermoelectric devices (e.g., light-emitting diodes, transistors, Seebeck generators), but even quantum light sources and related circuitry.

15:15	**Discussion on academic career path**
	with Prof. Dr. Andreas Rademacher / Prof. Dr. Gordon Callsen

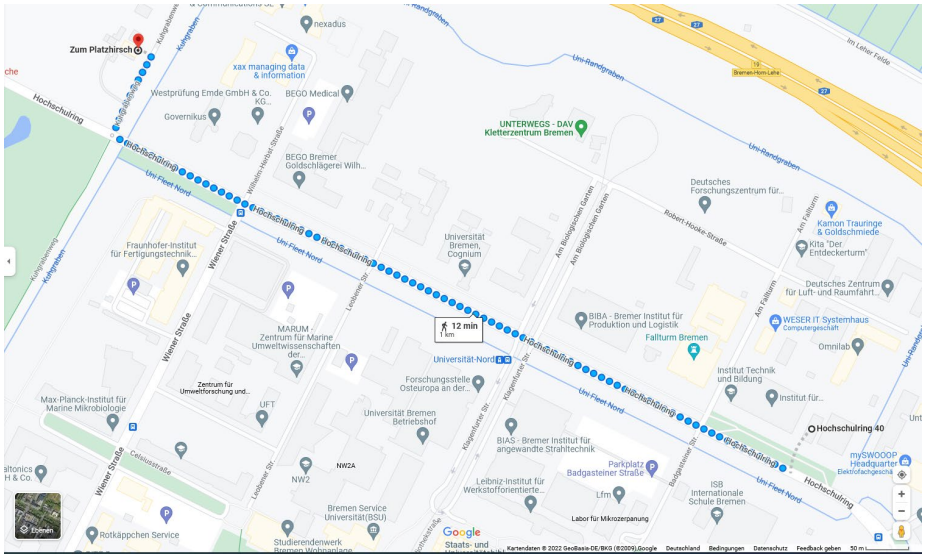
15:45	**General discussion / Coffee break**

16:00	**End of Workshop**

Get together / Social event

17:00 **Minigolf** („Zum Platzhirsch“, Kuhgrabenweg 30)

18:00 **Dinner** (“Zum Platzhirsch”, at your own expense)



Organizing committee

Enis Bicer, Hanna Lührs, Lena Ehlers

Support: Britta Hinz, Vanessa Röttger, Subrina Jahan, Bastian Dincher (photography)

MAPEX
Doctoral Qualification Programme

MAPEX seeks to support doctoral students in their personal development of professional and interdisciplinary skills and competences. Therefore, MAPEX provides a milestone-based programme that covers a comprehensive set of different qualification areas.

The MAPEX Doctoral Qualification Programme (MAPEX-QP) offers the following benefits to its participants:

- Receive a transcript of records summarizing all your achieved qualifications.
- Individual consultation and support with regard to your doctoral process and your personal competence objectives.
- A comprehensive overview about training courses and workshops offered by various institutions at the University of Bremen.
- Take part in workshops organized by MAPEX and the QP, which are specifically designed and oriented towards early career researchers.
- MAPEX funding opportunities promoting research activities and projects (see next page).

Contact and more information:

MAPEX-QP

MAPEX
Core Facility for Materials Analytics

A unique combination of cutting-edge instruments for the structural and chemical characterization of materials is being established within the University of Bremen by MAPEX in the form of the MAPEX Core Facility for Materials Analytics (MAPEX-CF).

As a user facility, the MAPEX-CF allows scientists from several disciplines to share and access a wide range of high-performance scientific equipment in the *investigation areas* of Electron Microscopy, 3D Materials Analytics, Surface Analytics, X-ray Diffraction, and Spectroscopy.

Funding

MAPEX, the MAPEX-QP and the MAPEX-CF support Early Career Researchers by providing funding for short-term research projects, materials analysis, workshops, and more.

Contact and more information:

MAPEX

MAPEX-CF

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5. **Thiemo Benthien,** 4 Production Engineering, University of Bremen
6. **Enis Bicer,** MAPEX, University of Bremen
7. **Ingmar Bösing,** 4 Production Engineering, University of Bremen
8. **Joshua Budde,** Fraunhofer IFAM
9. **Gordon Callsen,** 1 Physics / Electrical Engineering, University of Bremen
10. **Jan Yorrick Dietrich,** 4 Production Engineering, FIBRE
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37. **James Ziemah,** Constructor University Bremen

NOTES

Universität Bremen

MAPEX Center
for Materials and Processes

15th MAPEX Early Career Researcher Workshop

With the aim of “building bridges” across faculties and institutes we encourage early-career researchers to boost their careers through interdisciplinary exchange.

The workshop is a good platform for you if you would like to …

- get in touch with peers, build up your own network of experts,
- learn from others, think outside the box,
- open doors to other experts – become aware of the huge potential for mutual support that you can access on the short way,
- develop ideas for cooperative research projects,
- get to know how MAPEX and the MAPEX Core Facility can support your research.

University of Bremen
MAPEX Center for Materials and Processes
www.uni-bremen.de/mapex