Universität Bremen

MAPEX Center
for Materials and Processes

PROGRAMME

13th MAPEX Early Career Researcher Workshop

BUILDING BRIDGES
across the borders defined by the faculties and institutes

26th April 2022

13 MAPEX Materials Methods Technologies
Early Career Researcher Workshop

MAPEX Bremen

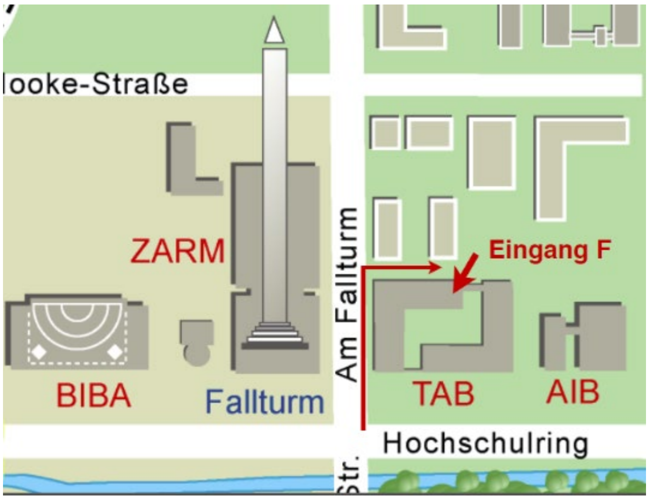
Programme overview

26th April 2022

8:30	**Registration and poster mounting**
9:00	**Welcome and introduction**
9:15	**Session 1**
10:15	**Coffee break**
10:30	**Session 2**
11:30	**Poster session and lunch break**
12:30	**Session 3**
14:20	**Poster session and coffee break**
15:00	**Session 4**
15:45	**Coffee and networking**

	Get together
17:00	**Minigolf** (Zum Platzhirsch, Kuhgrabenweg 30)
18:00	**Dinner** (Zum Platzhirsch, at your own expense)

Venue



AIB building

Hochschulring 40

First floor

Session 1

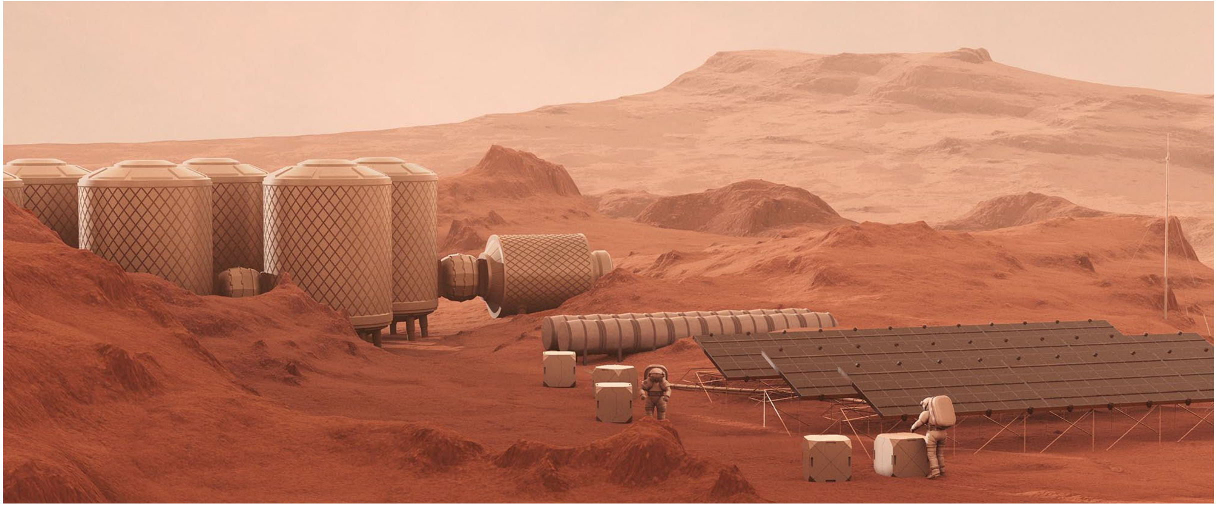
09:15 Where do we want to go? The MAPEX contribution to sustainable human Mars exploration

*Christiane Heinicke**
ZARM, University of Bremen

Leading space agencies intend to bring humans to Mars in the next decades, with some private companies pushing for sooner deadlines. In fact, promises and plans to land humans on Mars have recurrently been announced since the end of the Apollo era, but have remained largely incomplete or even abandoned. At the University of Bremen we are convinced that human Mars exploration will happen and that it will have a huge impact on both humankind and on the Martian environment. Given that even optimists do not see humans on Mars before the 2030s, we believe that now is the right moment to research possible scenarios for human Mars exploration and settlement, and to study the consequences for Earth, Mars and humankind.

To this end, MAPEX has formed the new research initiative "Humans on Mars" (working title) with the support of the University of Bremen and the State of Bremen. Since our approach to human Mars exploration is transdisciplinary and human-centered, MAPEX researchers are joined by researchers in the field of human and social sciences at the University of Bremen. We here argue that human Mars exploration can be instrumental in leading a change from a technology-centered toward a human-centered society, thereby solving our most pressing problems on Earth.

In this talk, we will first outline our general approach to combining the technological with the societal challenges. We will then present concrete examples, including some past and future experiments that were and will be conducted in the MaMBA-laboratory at the ZARM.



* co authors: Marc Avila, Christiane Heinicke, Lucio Colombi Ciacchi, Armin Dekorsy, Sebastian Fehrler, Hanna Lührs, Kurosch Rezwan, Norman Sieroka, Kirsten Tracht

09:45 Flashlight presentations 1

P01 Ultrastructure and biomechanics of starfish ossicles

Raman Raman
Hochschule Bremen

Starfish's endoskeleton is formed by many intricate bone-like structures (ossicles) which are connected to each other with small muscle tissues and embedded in a collagenous matrix. The ultrastructure of these ossicles shows the presence of a porous microstructure (stereom). To investigate whether the morphology of this ultrastructure is correlated with biomechanical stresses, we analyzed and compared the stereom patterns found in different types of ossicles in Asterias rubens.

P02 Mechanical stress on insect exoskeleton

Karen Stamm
Uni Bremen (FB2), Hochschule Bremen

For the second most common biological material worldwide, insect cuticle, it is so far unknown if and how it reacts to long-term higher mechanical stress. We present our first results of increased mechanical stress on the exoskeleton using a novel staining method to visualize its main components, exo- and endocuticle, in µCT scans (XRM).

P03 The Living Habitat

Ksenia Appelganc, Saurabh Band & Paul Groeβe Maestrup
University of Bremen

In our project "The Living Habitat" we aim to integrate a photobioreactor (PBR) into the MaMBA habitat laboratory at ZARM as a component of a life support system. The PBR should revitalize the air and adapt to oxygen requirements. For monitoring the PBR, we plan to develop interactive sensor networks. The PBR and sensor networks will function autonomously as an artificial agent as part of the living habitat. We want to present initial ideas and our different interdisciplinary approaches.

P04 Comparing Thermal Stability between Phosphonic Acid- and Thiol-Anchored SAMs

Andika Asyuda
FB 01, University of Bremen

The issue of thermal stability of functional SAMs on coinage metal and oxide substrates was addressed. This issue is of a crucial importance for applications, defining the temperature range of SAM-based devices and framing the preparation routes involving high temperature steps. Several representative SAMs with thiol anchoring group on Au(111) substrates and phosphonic acid (PA) anchoring group on Al_2O_3 substrates were studied by high resolution X-ray photoelectron spectroscopy.

P05 Modeling of Electrochemical Oxide Film growth

Ingmar Bösing
FB 04, University of Bremen

Oxide film growth is modeled by interfacial reactions and transport of crystal defects and electrons and holes through the film. By the simulation the properties of the oxide can be derived and the polarization behavior of metal electrodes covered by an oxide film can be decribed.

P06 Cellophane as an alternative separator for MEC operation with anaerobic digester effluent

Simone Colantoni
FB 04, University of Bremen

Microbial electrolysis cells (MEC) are a novel technology that couples wastewater treatment with energy recovery in the form of hydrogen. The state-of-the-art separators commonly utilized are expensive ion-exchange membranes. The aim of this work is to identify the suitability of low-cost cellophane-based materials as separators for a MEC working with the effluent of an anaerobic digestor.

10:00 Data Train
Training in Research Data Management and Data Science

*Tanja Hörner**
U Bremen Research Alliance

Data-driven science is becoming increasingly important in answering the pressing research questions of our time. Global warming, massive extinction of species and the impact on human health as well as the socio-economic consequences of the COVID-19 pandemic are just some recent examples. However, there is a significant deficit of qualified persons in (research) data management and data science to foster innovative "Big Data" technologies for science and the private sector worldwide. Responding to this massive demand, the U Bremen Research Alliance [1], with the support of the Federal State of Bremen, has established the cross-institutional and cross-disciplinary training program "Data Train - Training in Research Data Management and Data Science" [2] for doctoral researchers from member institutions. Data Train pursues the mission of strengthening the competencies in data literacy, data management, and data science, while offering doctoral researchers a platform to build an interdisciplinary and interinstitutional network.

The program is associated with the German National Research Data Infrastructure (NFDI) [3]. NFDI consortia represented in Bremen (NFDI4Health, NFDI4Biodiversity, KonsortSWD, NFDI4Ing, NFDI4DataScience, NFDI4Earth, NFDI-MatWerk, NFDI4Microbiota) participate in the development and operation of the training courses. In 2021, the program was piloted with a total of 40 lecturers, 29 lectures and 222 doctoral researchers participating. Moreover, since the program was offered virtually, more than 1,600 participations were registered. Starting in 2022, the program will be offered annually. The cross-institutional and cross-disciplinary training model covers the entire data value chain and makes an important contribution to data literacy training which is beneficial for science as well as for the private sector.

[1] The University of Bremen and twelve federal and state financed non-university research institutes cooperate within the U Bremen Research Alliance. The Alliance includes research institutes of the four major German science organizations, i.e. Fraunhofer Society, Max Planck Society, Leibniz Association and Helmholtz Association, as well as the German Research Center for Artificial Intelligence. (https://www.uni-bremen.de/research-alliance)
[2] https://bremen-research/data-train/
[3] In the National Research Data Infrastructure Germany (NFDI), valuable data from science and research are systematically accessed, networked and made usable in a sustainable and qualitative manner for the entire German science system. (https://www.nfdi.de/)

*co-authors: Frank Oliver Glöckner, Rolf Drechsler, Iris Pigeot

Session 2

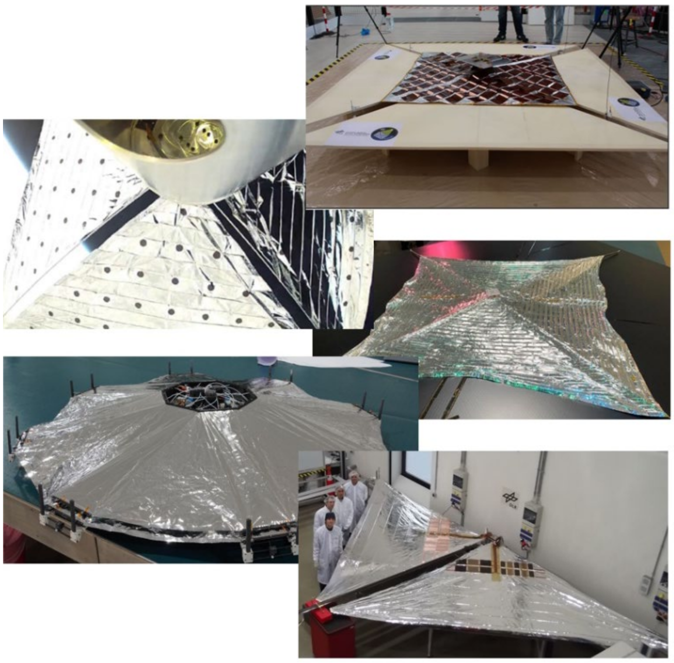
10:30	Thin-film materials in Space

Patric Seefeldt
DLR Institute of Space Systems

In receent projects we investigated coated polyimide and fluorpolymer thin-films for Low Earth Orbit (LEO) applications such as drag sails and flexible solar arrays. Atomic Oxygen (AO) errosion and resistance agains Ultraviolet (UV) radiation are the most critical aspects in the selection and design of such materials.

Several material candidates were selected for different projects or applications, respectively. Subtstrate materials are polyimide, black polyimide and fluorpolymers. These are coated with comibinations of polysilazane, silicon oxyde, aluminum and indium tin oxide. By exposing these materials to the space environment and analysing the mass loss as well as using optical spectroscopy and microscope analysis the material aging is studied.

Some of the materials were subject to of laboratroy AO tests at ESA/ESTEC, some are currently on the International Space Station as part of the Materials International Space Station Experiment (MISSE-14) and we have prepared samples for the ESA's Euro Material Ageing experiment which is planned to be exposed on the Bartolomeo platform of the International Space Station (ISS) in the next year. In the paper the analysis behind the material selection will be discussed and first results from laboratory tests will be presented.



11:00 Flashlight presentations 2

P07 Screening of microbial electrolysis cell bioanodes for brewery wastewater treatment

Marcos Isaac Vázquez Sánchez
FB 04, University of Bremen

The constantly changing conditions of wastewater make the selection of anode materials for microbial electrolysis cells difficult. This work focuses in the simultaneous testing and selection of six anode materials in realistic poorly buffered and low-conductivity brewery wastewater media. Under these conditions stainless-steel EN 1.4113 obtained a limiting current density of 0.45 ± 0.07 mA·cm 2, 28.8 % higher than previous works with other stainless-steel wool electrodes in acetate media.

P08 NMR characterization of mass transfer in hierarchical porous catalysts for FTS

Alexander Zimmermann
FB 04, University of Bremen

The Fischer-Tropsch synthesis (FTS) is a key technology for a future circular economy. However, it often suffers from mass transfer limitation, against which hierarchically porous catalyst pellets offer great potential. I investigated such samples using a combination of NMR methods, first-time taking emulsification effects of reaction products into account. The results uncovered a new potential benefit of these pellets, namely eliminating transport resistances of emulsion phase boundaries.

P09	**Green electrochemical synthesis of oxygen and metals from regolith**

Reza Fayaz
FB 04, University of Bremen

The plan to establish a colony on Mars, with the huge demand for construction materials and oxygen as life support, could only be plausible through the advancement of in situ processes. The top loose layer of soil on Mars (regolith), composed of various metal oxides, could be a reach resource in this respect.

P10	**MRI as a quantitative method for characterization and optimization of live electroactive biofilms inside porous electrodes**

Luca Häuser
FB 04, University of Bremen

Information about electroactive biofilms (EAB) is required to obtain a deeper understanding of limiting processes & to develop improved porous electrodes. Magnetic Resonance Imaging (MRI) characterizes EABs in porous, opaque electrodes regarding: Structure (T1 & T2), Reaction (CEST & 31P MRSI) & Transport (diffusion & perfusion imaging). Complementary methods like X-ray microscopy, fluorescence microscopy, qPCR & protein quantification will validate determined biofilm parameters.

P11	**Computational study of energy level alignment at the interface of PTCDA/CeO2 heterojunction**

Chieh-Min Hsieh
FB 02, University of Bremen

Rational design of hybrid solar cells relies on clear understanding of energy level alignment (ELA) of materials at interfaces, which influences the functionality and performance of hybrid solar cells. My current work focuses on density functional theory (DFT) computation of ELA at the interface of perylenetetracarboxylic dianhydride (PTCDA) and CeO2. Using quasiparticle GW approximation implemented in BerkeleyGW code, the energy level of PTCDA/CeO2 system can be calculated.

P12 **Synthesis and reaction of a new aminoterminated hyperbranched polyglycerol with polyethylene glycol dialdehyde to an imine-crosslinked hydrogel**

Kyriakos Karakyriazis
FB 02, Fraunhofer IFAM

The objective of this research is to synthesize a biodegradable bone adhesive hydrogel, to provide a better alternative to the classic osteosynthesis materials (nails, screws, plates, wires), avoiding the need of a second operation. A new aminoterminated hyperbranched polyglycerol was synthesized for this purpose. The aminoterminated hyperbranched polyglycerol reacted with PEG-dialdehyde, yielding imine-crosslinked hydrogels, which were characterized regarding their stability.

P13 **Extensive Proton Spectra for Interplanetary Space**

Erik Klein
DLR, FB 04, University of Bremen

Man-made satellites are exposed to vacuum, electromagnetic and corpuscular radiation in space. In order to assess the possible effects of protons on functional surfaces, human crew and devices, an extensive spectrum is needed. In order to fill gaps and to summarize models, an extensive spectrum is introduced. This will enable the user to quickly assess the entire energy range and extract the information he needs for his application, such as dose calculation or surface alteration.

11:15 **MAPEX Doctoral Qualification Programme**

Enis Bicer
MAPEX, University of Bremen

MAPEX offers a Doctoral Qualification Programme that aims to prepare young scientists for future leadership positions in industry and academia and to support them during their PhD. I will present details and benefits of participating in the programme.

Session 3

12:30	**Tuning material properties by correlated disorder**

Ella Schmidt
FB 05, Crystallography and Geomaterials, University of Bremen

When the structure of a material is known, we can calculate its physical properties, such as the compressibility, the electronic band structure and lattice dynamics. For completely ordered materials, structure determination is a routine process and the physical properties are easily accessible. As soon as the material shows disordered components, structure determination is more complex and the calculation of physical properties usually involves the so called "virtual crystal approximation": For a very simple model system, e.g. KBr_xCl_{1-x}, physical properties would be approximated as the weighted average of the properties of KBr and KCl.

In many disordered materials the distribution of the disordered components is far from random: Certain atomic arrangements may be preferred and the locally different chemical environments lead to bond-distance relaxations; hence local atomic configurations differ significantly from the average structure. These local correlations influence the physical properties and therefore tuning local correlations allows to tune physical properties.

By means of single crystal diffuse scattering analysis we investigate the simple rock-salt structured model system KBr_xCl_{1-x}. We show how the lattice dynamics are influenced by correlated disorder and discuss how this approach could be used to tailor thermoelectric materials.

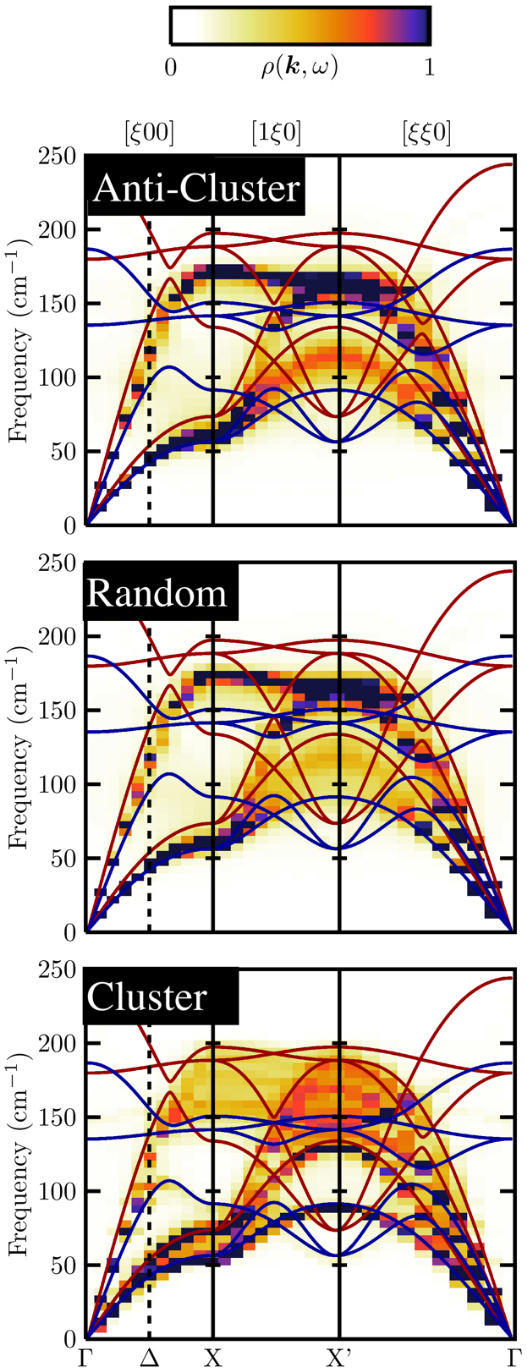


Figure: Phonon dispersion curve of $KBr_{0.5}Cl_{0.5}$ compared to KCl (blue) and KBr (red). The dispersion changes significantly if likewise anions are anti-clustering, distributed randomly or clustering.

13:10 Organic Mixed Ion/Electron Conductors: From Organic Electrochemical Transistors to Highly Sensitive Biosensors

Björn Lüssem
FB 01, University of Bremen

Organic materials that transport ionic and electric charge equally well[1] enable completely new design principles for electronic devices and are at the heart of various novel organic devices[2] such as highly sensitive organic biosensors or neuromorphic devices . In particular, the strong coupling between ion and charge transport observed in these organic mixed conductors has made them a key driver in novel organic bioelectronics based on Organic Electrochemical Transistors (OECTs), with technological demonstrations that include in-situ measurements of brain activity, collection of electrocardiograms, and the tracking of eye movement[3] .

In this presentation, the physics of Organic Electrochemical Transistors is reviewed. Current bottlenecks for device optimization are summarized[4], stressing the need for advanced two-dimensional device modeling and a targeted design of improved semiconductors, electrolytes, and contact materials[5].

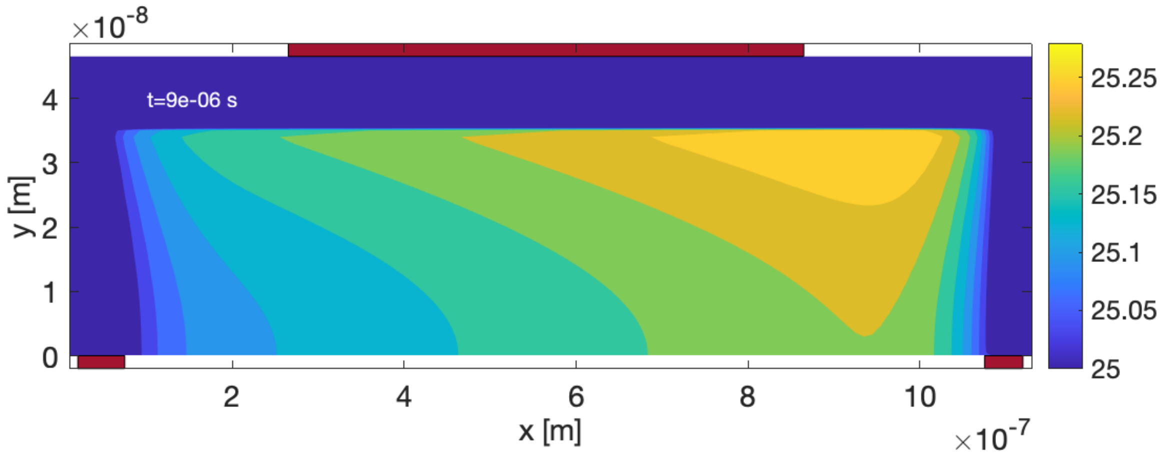


Figure: Snapshot of the concentration of cations during the turn-off of an organic electrochemical transistor.

[1] B. D. Paulsen et al., *Nat Mat* 19, 13-26, (2020).
[2] J. Rivnay et al., *Nat Rev Mater* 3, 17086, (2018); X. Strakosas et al., *J Appl Polym Sci* 132, (2015).
[3] P. Leleux et al., *Adv Health Mater* 4, (2015).
[4] Kaphle, Lussem et al., *Nat Comm* 11, 2515, (2020); Paudel, Lussem et al., *Adv Func Mat* 31, 2004939, (2021)
5 Paudel, Lussem et al., *J Mat Chem C* 31, 9761, (2021)

14:10 Flashlight presentations 3

P14 Design of a ceramic/polymer cell for harvesting proton radiation in extra-terrestrial environments

Tanja Link
FB 04, Uni Bremen, Fraunhofer IFAM

The overall project aims to develop new types of materials for space travel, which will protect against ionising space radiation, measure radiation exposure and convert its inherent energy into electricity. Here, we demonstrate first steps to develop a thin cell that interacts with proton radiation to generate electricity. The investigated principle is based on a semiconductor junction and the specific interaction of ceramic nanoparticles with ionising radiation.

P15 Organic modification of layered silicates as barrier pigment in coating systems

Joshua Lommes
FB 02, Fraunhofer IFAM

Organic modification of layered silicates coordinated to the polymer matrix Improving the exfoliation of layers Processing in different coating systems Reducing the permeation velocity of water vapour and gases

P16 Pinpointing Hubbard corrections to tackle inhomogenous nl subshells: The DFT+U(m) method

Eric Macke
FB 04, University of Bremen

DFT+ U remains a key tool in computational material science as it mitigates the DFT self-interaction error. While this approach often provides good electronic and magnetic properties, recent investigations revealed that DFT+ U over-stabilizes high spin configurations of transition metal elements surrounded by strong ligand fields. Here, we propose a more flexible scheme that enables the use of distinct Hubbard parameters U(m) for the same species, computable by means of ab initio methods.

P17 Salt-induced fibrillogenesis of fibrinogen

Aparna Sai Malisetty
FB 04, University of Bremen

Fibrinogen is a blood plasma protein and converts to fibrin during blood clotting. In our previous work, a new routine for salt-induced fiber formation of fibrinogen is presented. However, the cause of this fiber formation is not known. Therefore, the goal of my research is to understand the effect of salt ions on fibrinogen fiber formation and its structure using MD simulations.

P18 Electrochemical impedance spectroscopy for the characterization of biofilms in bioelectrochemical devices

Óscar Santiago Carretero
FB 04, University of Bremen

In-situ characterization of electroactive biofilms is a great challenge in the study of bioelectrochemical systems. In this context, electrochemical impedance spectroscopy (EIS) arises as a promising technique due to its low interference with the operation of the system. This work explores the use of EIS to track the status of a bioanode in a microbial electrolysis cell. The results show a progressive decrease of the total impedance from more than 1800Ω to below 20Ω, over a period of 3 weeks.

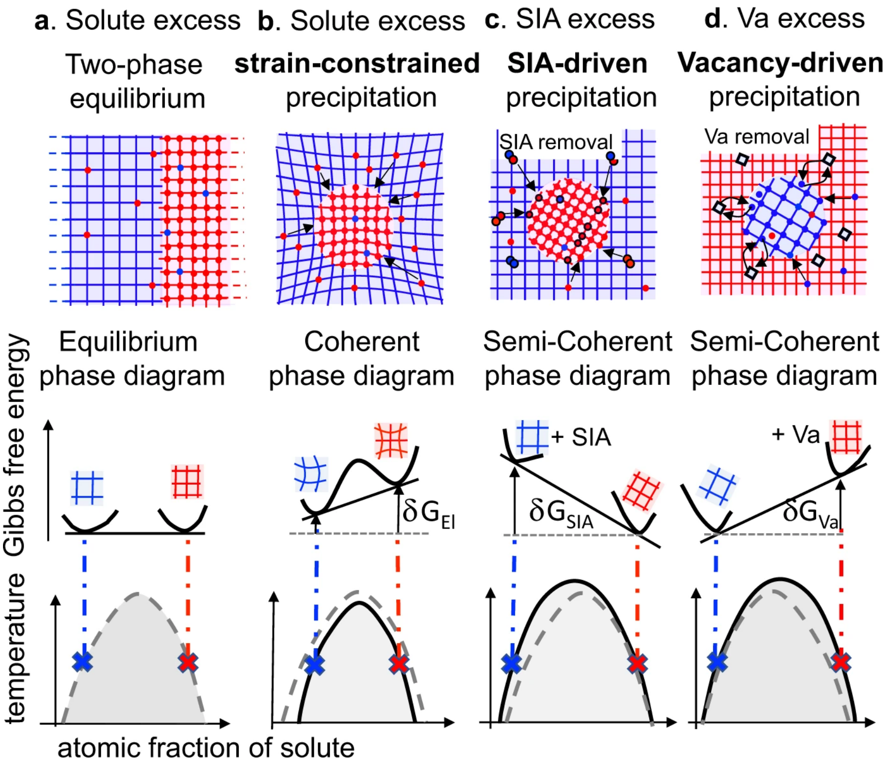
15:00 From atomic diffusion acceleration to phase transformation : the contribution of atom probe tomography

Lisa Belkacemi
Leibniz-Institut für Werkstofforientierte Technologien-IWT

Secondary phase precipitates contribute to the microstructure of a material. The energy barriers that the system needs to overcome to reach its equilibrium are reduced through well-known accommodation mechanisms (elastic deformation, dislocation diffusion).

In this presentation, I will first lay out a joint experimental and modeling study based on the characterization of an undersaturated Fe-3at.%Ni model alloy using high resolution transmission electron microscopy (HR-TEM) and atom probe tomography (APT). The material of interest was irradiated with Fe ions, triggering the formation a secondary phase that was not predicted by the Fe-Ni phase diagram. Linking the phase chemistry, the phase proper strain (eigenstrain or stress-free strain) and the excess concentration of point defects revealed the existence of a novel accommodation mechanism [1].

Secondly, I will give the example of intrinsic heat treatments (IHT) generated during laser metal deposition (LMD). The microstructure evolution of the 3D printed X40CrMoV5-1 steel was investigated by in-situ High Energy X-Ray Diffraction (HEXRD) experiments (DESY Synchrotron, Hamburg). The nano-precipitates identified during the LMD process were characterized by APT, unveiling the presence of diverse nanoprecipitates' populations and giving new insights into carbon partitioning during the martensite formation and subsequent (self-)tempering. [1] M. Nastar et al., Nature Com. Mat. 2, 32 (2021).



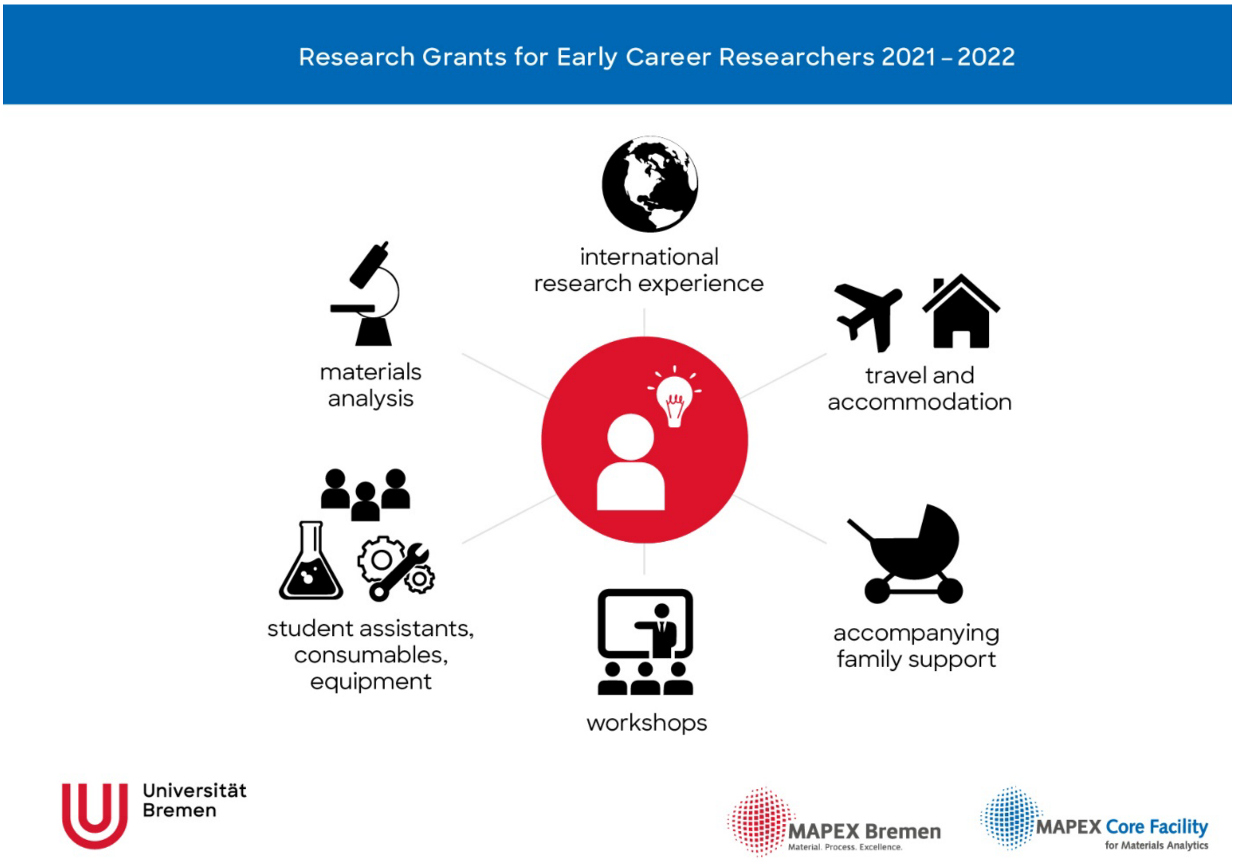
Illustrations of (a) the final equilibrium state between infinite volume phases (blue and red domains), (b) a deformed precipitate (in red) in a supersaturated solution, with an elastic strain ensuring the continuity of the lattice at the precipitate/matrix interface, and reducing the two-phase domain of the phase diagram; (c, d) the semi-coherent precipitation in an undersaturated solid solution triggered by respectively an excess of self-interstitial atoms (SIA) and an excess of vacancies (Va).

15:30 How the MAPEX Core Facility for Materials Analytics supports your research

Guilherme Dalla Lana Semione

FB 04, University of Bremen

The MAPEX-CF is a shared materials analysis and characterization facility that offers research services for both university-internal and external users. It comprises five investigation areas: 3D Materials Analytics, Electron Microscopy, Surface Analytics, Spectroscopy, and X-ray Diffraction. Here it will be shown the current status and prospects of the project and how it can impact the research performed at the University of Bremen.



Get together

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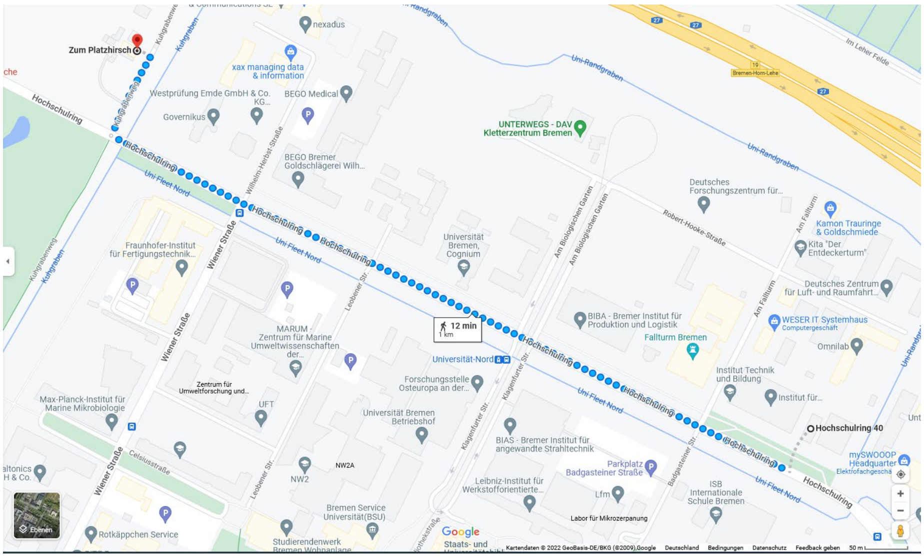
18:00 **Dinner** (Zum Platzhirsch, at your own expense)



Organizing committee

Hanna Lührs

Britta Hinz

Enis Bicer

Guilherme Dalla Lana Semione

Jan Eggert

Bastian Dincher (photographer)

Participants

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2. **Ksenia Appelganc**, FB 07, University of Bremen
3. **Andika Asyuda**, FB 01, IMSAS, University of Bremen
4. **Saurabh Band**, FB 01, University of Bremen
5. **Lisa Belkacemi**, Leibniz IWT
6. **Enis Bicer**, MAPEX, University of Bremen
7. **Ingmar Bösing**, FB 04, University of Bremen
8. **Simone Colantoni**, FB 04, University of Bremen
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22. **Vincent Hock**, FB 01, University of Bremen
23. **Tanja Hörner**, U Bremen Research Alliance
24. **Chieh-Min Hsieh**, FB 02, University of Bremen
25. **Muchammad Izzuddin Jundullah Hanafi**, FB 02, University of Bremen
26. **Kyriakos Karakyriazis**, FB 02, Fraunhofer IFAM
27. **Md KARIM**, FB 04, University of Bremen
28. **Erik Klein**, DLR, FB 04, University of Bremen
29. **Tanja Link**, FB 04, Uni Bremen, Fraunhofer IFAM
30. **Joshua Lommes**, FB 02, Fraunhofer IFAM
31. **Hanna Lührs**, MAPEX, University of Bremen
32. **Björn Lüssem**, FB 01, IMSAS, University of Bremen
33. **Eric Macke**, FB 04, University of Bremen
34. **Aparna Sai Malisetty**, FB 04, University of Bremen
35. **Govindarajan Prakash**, FB 01, University of Bremen
36. **Raman Raman**, Hochschule Bremen
37. **Saman Razavi**, Fraunhofer IFAM
38. **Kurosch Rezwan**, MAPEX Speaker, University of Bremen
39. **Óscar Santiago Carretero**, FB 04, University of Bremen
40. **Tarek Scheele**, FB 02, University of Bremen
41. **Ella Schmidt**, FB 05, University of Bremen
42. **Patric Seefeldt**, DLR Institute of Space Systems
43. **Michael Skowrons**, FB 01, University of Bremen
44. **Karen Stamm**, Uni Bremen (FB2), HS Bremen
45. **Maciej Sznajder**, DLR Institute of Space Systems
46. **Marcos Isaac Vázquez Sánchez**, FB 04, University of Bremen
47. **Alexander Zimmermann**, FB 04, University of Bremen
48. **Hannah Zindel**, MAPEX, University of Bremen

NOTES

13th 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