MAPEX Bremen

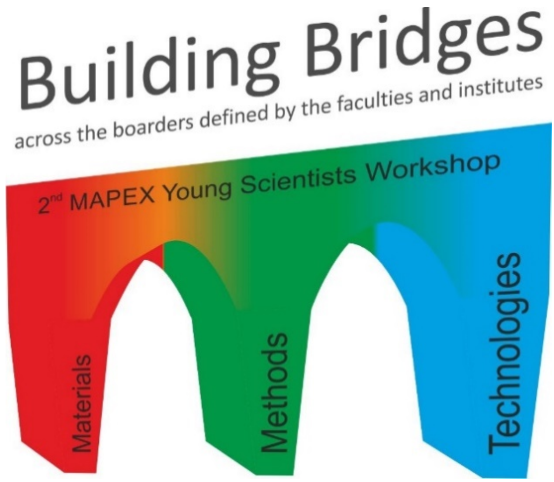
Material. Process. Excellence.

2nd MAPEX Young Scientist Workshop

PROGRAM

April 11th, 2016

TAB Building



Universität Bremen

2nd MAPEX Young Scientist Workshop

	Overview
8:00	Registration and Poster Mounting
8:30	Session 1
10:00	Coffee Break
10:15	Session 2
11:30	Poster Session 1
12:30	Lunch Break
13:30	Session 3
15:00	Poster Session 2
16:00	Plenary Lecture
17:00	End of Workshop
18:00	Social Event (Schwarzlichthof)

Session 1

8:30 Welcome note from MAPEX speaker

Lucio Colombi Ciacchi, FB4, MAPEX

8:45 Introduction to MAPEX, Instrument Database, Program

Hanna Lührs, MAPEX

9:00 Atomistic Modelling of Porous Solids - From Fundamental Understanding to Applications

Michael Fischer, FB5, Crystallography

This contribution will present illustrative examples from our computational studies of adsorption in crystalline porous materials (focusing on zeolites). After a brief overview of the materials and methods, examples will include force-field based Monte Carlo simulations of gas separation, and density-functional theory studies of water adsorption. In particular, it will be discussed how computational chemistry methods can improve our understanding of the interactions that govern adsorption.

9:30 Lightning Presentations

L1 Aminosilane - Virus Interactions in a Functionalized Ceramic Membrane

Nils Hildebrand, FB4, BCCMS

A recently developed aminosilane functionalized ceramic membrane showed a high ability to retain the model virus MS2. We suggest three types of possible interactions. (1) The binding of the positively charged aminosilanes through pores in the virus capsid to reach the negatively charged genome. (2) An adsorption of aminosilanes to expressed binding specific surface groups on the coat proteins. (3) A very selective interaction to the maturation protein embedded asymmetrically in the capsid.

L2 Biomineralization of iron oxyhydroxides on individual ferritin units supported on (bio)silica

Steffen Lid, FB4, Hybrid Materials Interfaces Group

We employ individual Ferritin subunits as a template for continuous 2D films, supported on multidimensional oxide scaffolds, by the covalent immobilization of individual Ferritin subunits on chemically and thermally stable templates, such as (bio)silica. A sophisticated combination of experimental and atomistic modelling techniques enable us to develop a material-design protocol based on fundamental physical/chemical knowledge of the investigated biomineralization system.

L3 A new discrete element contact model to simulate the mechanical behaviour of TiO_2-nanoparticles in films and aggregates

Jens Laube, FB4, BCCMS

We use extensive all-atom molecular dynamic simulations and force spectroscopy experiments to investigate the forces between nanoparticles under ambient conditions. The insights from these findings are then incorporated into the discrete element modeling method to investigate the mechanical behaviour of large nanoparticle films in dependence on ambient conditions, film porosity and connectivity.

L4 Injection moulding simulation of natural fibre-reinforced polymers

Katharina Albrecht, Hochschule Bremen - Fachrichtung Bionik

Due to growing environmental concerns natural fibre (NF)-reinforced, injection moulded (IM) polymers are an interesting prospect for many applications. As engineers only consider predictable compounds in component development processes, models to simulate NF compounds need to be developed. A first model for NF-reinforced PP was developed to simulate automotive components. Here the transferability to a non-automotive tool (sand moulds) shall be shown, validating the IM simulation by experiments.

L5 Modelling of the mechanical properties of flax fibre-reinforced composites - Predictability of fibre and composite properties

Katharina Haag, Hochschule Bremen - Biomimetics

The scatter in natural fibre properties is known as a bottle neck for their acceptance as reinforcement in structural applications. We show the influence of the fibre properties on the composite performance. Calculation models are applied and show that the properties of flax - reinforced composites can be predicted well and that the scatter of composite properties is much lower than that of fibres. We propose to calculate the reinforcing potential of the fibres based on the composite properties.

L6 Model based correction of tool paths

Arne Bloem, FB4, bime

Model based compensation can increase the dynamic of feed axis while maintaining a consistent accuracy. Especially in the domain of ultra precision manufacturing this is beneficial, since the manufacturing processes are very slow and time consuming. However, this requires a model that satisfies the high requirements of ultra-precision machining. To meet the requirements an adaptive model is developed that adjusts its parameters continuously.

10:00 Coffee break

Session 2

10:15 Material-integrated intelligent systems: Challenges and Perspectives

Dirk Lehmhus, FB4

As technical vision inspired by natural examples like human skin, material-integrated intelligent systems are a highly cross-disciplinary topic. Ultimately, these sensorial materials will be processable like today’s semi-finished ones, adding sensing and information processing. To achieve this, they must be heterogeneous, incorporating sensors, microelectronics, power supply and communication. Though these elements exist, few of them are optimized for material integration. The talk outlines status and trends, highlighting Bremen research contributions.

10:45 Lightning Presentations

L7 Ultra precision balancing of air bearing spindles during rotation

Eike Foremny, FB4

In order to cut surfaces in optical quality air bearing spindles are used. These must be precisely balanced to achieve the required true running accuracy as well as to avoid damaging the air bearings. In this project a balance system based on the rotational redistribution of mass is developed. The required torque to shift the balance masses is generated by an ultra sonic motor. The system is able to rotary shift balance masses while mounted on a operating spindle.

L8 Thermal issues of rotary swaging

Yang Liu, FB4, bime

During rotary swaging the local temperature can be high enough to affect the material properties. Better understanding of the thermal issues and improvement of forming performance are needed. The sources and sinks of heat and their influences are considered.

L9 Micro Applications of Electromagnetic Forming

Lasse Langstädtler, FB4, bime

Electromagnetic forming is a high speed forming process where one part of the tool is replaced by a strong electromagnetic field. This field generates a contactless working force on the sheet. The major advantage is the very high deformation rate which leads to higher plasticity of the sheet metal material and shorter cycle times. The challenge of forming thin sheet metals is the decreasing of body forces and the local heating by eddy currents that can melt or even vaporize the material. The aim is to overcome the challenges for micro applications like micro embossing, cutting and joining.

L10 Potentials of Dry Rotary Swaging

Marius Herrmann, FB4, bime

Rotary swaging is a cold bulk forming process. The established processes use lubricants which fulfill necessary functions such as lubricating, cooling and cleaning of the tools. Disadvantages caused by lubricant are costs of recycling, replacement of lost coolant and for the cleaning of the workpiece. To eliminate the lubricant it is necessary to substitute the functions in other ways. A straight way forward to cope with this challenges is the combination of coating and structuring of the tools.

L11 Process combination of rotary swaging and extrusion

Svetlana Ishkina, FB4, bime

Micro rotary swaging is a cold forming process which changes the microstructure of the workpiece material. This project aims at an improvement of the material properties of the swaged parts for further forming operations such as extrusion. For this purpose the geometry of the dies and the process kinematics are adapted.

L12 Multi-Slip 3D Continuum Dislocation Dynamics Simulations of Dislocation Structure Evolution in Bending of a Micro-Beam

Alireza Ebrahimi, FB4, Werkstoffmechanik - Computational Material Modeling

A persistent challenge in multi-scale modeling of materials is the prediction of plastic materials behavior based on the evolution of the dislocation state. An important step towards a dislocation based continuum description was recently achieved with the so called continuum dislocation dynamics (CDD). The lowest order closure of CDD employs three internal variables per slip system, namely the total dislocation density, the classical dislocation density tensor and a so called curvature density.

L13 Preparation and Properties of inverse Nanoparticle–Polymer–Composite–Layers

Ron Hoffmann, FB2, IFAM

In contrast to conventional nanoparticle–polymer–composite preparation, the inorganic particle framework will be prepared prior to infiltrating it with the monomer followed by polymerization. The kinetics and physics will be evaluated and the monomer turnover will be determined. Cure shrinkage will be examined by various methods. The inverse composites possess great potential as a thin–film–layer for photo catalysis, water-splitting reactions and biological sensors in liquid environments.

L14 Methodology to indentify the machine settings in production processes

Marc Redecker, FB4, BIK - Institut für integrierte Produktentwicklung

Within a production process with different process steps materials are produced to a final product. The materials are liable to a strong variability relating to material quality and has a nominal-actual value difference. During the production process incorrectly machine settings lead to a further accumulation of variations in quality. The outcome of this is a final product with high quality variations. The question is which methodology can be used to identify the relationships between input parameters , machine parameters and final product quality.

Poster Session 1

11:30 Poster session and coffee break

Lunch Break

12:30 Lunch (Mensa)

Session 3

13:30 Materials science meets biology: Synthetic cell systems

Dorothea Brüggemann, Emmy Noether research group for nanostructured biomaterials, Institute for Biophysics, FB1

Biomedical applications ranging from tissue engineering to drug delivery systems require the development of versatile biomaterials and model systems, which can facilitate cell dhesion. We have recently established a minimal cell model to study cell adhesion with reduced molecular complexity. Using lipid vesicles with reconstituted adhesion proteins we were able to mimic cell adhesion on different extracellular matrix proteins. Further on, we introduced a novel extrusion approach to prepare biopolymer nanofibers, which mimic the extracellular environment. Ceramic alumina nanopores were used to extrude various biopolymers into nanofibrous scaffolds with reproducible fiber diameters. An important advantage of this method is the use of physiological buffers, which supports the biological functionality of our new biomaterials.

14:00 Lightning Presentations

L15 LifeChip - Seeding and feeding of mammalian cells

Frank Bunge, FB1, IMSAS

The LifeChip-Project aims at designing a microchip which enables the cultivation of mammalian cells. Cells will be seeded on specific spots , fed nutrition and oxygen and will be detached. Using hydrogels will create porous walls for the transport of nutrition as well as Parylene to manipulate the surface properties.

L16 Functional porous ceramics for biotechnological applications

Gesa Hollermann, FB4, Advanced Ceramics

Enzyme-based processes offer great potential for resource-efficient degradation of harmful substances. Porous Al_2O_3-SiO_2 carriers will be fabricated via ionotropic gelation of alginate, featuring hierarchically pore sizes, high surface area, high solvent stability. The influence between carrier features, surface functionalization, flow conditions and enzyme-specific properties will be addressed. The model enzymes catalase and glucoseoxidase perform sequential reactions which are easy to detect.

L17 Proteolytic ceramic capillary membranes for the preparative production of bioactive peptides

Marieke Hoog Antink, FB4

Bioactive peptides have a significant impact on the human metabolism and its regulation. To a great extent, these peptides and their source proteins have not been systematically identified and characterized yet. For the production of defined peptide fingerprints, protease-functionalized ceramic capillary membranes were used to hydrolyze a model protein under continuous flow conditions. A dependence of the obtained fingerprint on the applied flow rate was observed.

L18 Binding affinities and adhesion phenomena at the interface between binding peptides and zinc oxide

Monika Michaelis, FB4

This project will focus on the estimation of the binding affinities and adhesion phenomena like structural changes at the interface of binding peptides and zinc oxide via a combined approach of experimental and computational techniques and therefore will highlight the molecular nature of the interaction and elucidate the driving forces determining a peptide to be a specific binder.

L19 Growth of transition metal dichalcogenides on Ru(0001) and Si(111)

Moritz Ewert, FB1, Institute of Solid State Physics

Transition metal dichalcogenides (TMDCs) are known for their graphene-like electronically properties. Contrary to graphene, TMDCs possess a direct band gap, which allows TMDCs to be used as transistors, emitters, or detectors. Whereas most of the research uses exfoliated monolayers of TMDCs, this research is focusing on the epitaxial growth of tungsten disulfide and molybdenum disulfide under ultra-high vacuum (UHV) conditions. This approach allows the investigation of the chemical composition by X-ray photoelectron spectroscopy, the morphology by scanning tunneling microscopy and low-energy electron diffraction, and the growth process itself by low-energy electron microscopy.

L20 Identification of nanoscale phases using low energy electron microscopy by numerical I(V) analysis

Martin Hoppe, FB1, Institute of Solid State Physics

Low Energy Electron Microscopy (LEEM) is a method for investigating surface structures and morphologies. In LEEM crystal phases differing in sturcture or chemical composition may exhibit different intensities at a given energy. But, this does not allow for a definite identification especially on very heterogeneous surfaces. By numerical analysis and comparison of intensity-voltage I(V)-curves, which represent reliable fingerprints for each component, the identification and 2D mapping of the contributing surface phases is achieved.

L21 Growth, structure and morphology of NiGe and SnGe nanostructures on Ge(001)

Nicolas Braud, FB1, Institute of Solid State Physics

Nickel germanide is a promising candidate as a contact material in MOSFETs and is expected to play an important role in future Ge-based electronics due to its low formation temperature and low resistivity. In this context, SnGe can be used as channel material to improve the CMOS performance, as it has an even higher carrier mobility than Ge. Here we present an in-situ investigation of the growth of nickel germanide and SnGe at various temperatures on the Ge(001) surface by means of low-energy electron microscopy (LEEM) and micro diffraction (μLEED). We observe the growth of compact and elongated islands along two orthogonal directions after nickel deposition at 450∘C and 530°C. We also show that with increasing temperature, the size of the NiGe islands increases while the island density drastically decreases, showing an Arrhenius like behavior. Subsequent thermal annealing above 600°C results in the dissolution of the NiGe islands into the bulk substrate. Finally we compare the results obtained with the NiGe and those obtained with SnGe.

L22 Growth and characterization of thin vanadium dioxide films

Jon-Olaf Krisponeit and Simon Fischer, FB1, Institute of Solid State Physics

Vanadium dioxide exhibits a metal-insulator transition near room temperature, comprising a rich phenomenology that is still not fully understood. Close to the transition, the system responds sensitively to uniaxial substrate-induced stress, resulting in a wide variation of the transition temperature. In this contribution, thin VO_2 films were grown on $TiO_2(001)$ and $TiO_2(110)$ substrates by molecular beam epitaxy. Different growth methods were used: (1) vanadium evaporation under O_2 ambient, (2) cyclic vanadium deposition and post-annealing in O_2 and (3) cyclic vanadium deposition and oxidation with an oxygen plasma source . The prevalence of the V^{4+} oxidation state is confirmed by x-ray photoelectron spectroscopy (XPS). The surface structure is analyzed with low energy electron diffraction (LEED), indicating an epitaxial growth on the substrate and good crystallinity of the films. Scanning tunneling microscopy (STM) reveals continuous fllms of VO_2 on both substrates, we found faceting in the case of (110) substrate orientation, but terraces on (001) substrates.

L23 Influence of metal dopants on the catalytic properties of epitaxial rare earth oxide thin films

Simona Keil, FB2, IAPC

One strategy to improve activity and selectivity of metal oxide catalysts is to dope them with a second metal to generate new active centers. Previous studies have shown that methanol, water and CO show an intriguing chemistry on samaria films and islands epitaxially grown on Pt (111). In a new UHV study we aim at modifying and finally tuning the catalytic behavior of the samaria thin films by doping with palladium and titanium as low and high valence dopants.

L24 Selective oxidation of alcohols using unsupported highly porous gold as catalyst in liquid phase

Anastasia Lackmann, FB2, IAPC

Catalysis using gold has become popular due to its unique catalytic and chemical activity. Highly porous gold (npAu) material was discovered to be an active and stable catalyst in model experiments and gas phase catalysis. To understand its catalytic behavior in liquid phase catalysis, selective oxidation reactions of alcohols are ideally suited as a test reactions developing npAu as a green economically benign catalyst.

L25 Speckle-based 2D Sensor

Alexej Horosko, FB4

By using speckle correlation it is possible to calculate the displacement of two images with accuracy in the sub-pixel range. From images taken of moving surfaces the corresponding positions can be calculated with the speckle correlation. Furthermore due to the phenomenon of the Laser-Speckle on rough surfaces a pattern can be obtained that is suitable for precise measurements. The resolution and precision depends on the effective pixel-size and the characteristics of the images.

L26 Ultra-thin capacitive foil sensor for characterization of an adhesive joint

Martina Hübner, FB1, IMSAS

We present an ultra-thin capacitive foil sensor to monitor the curing of an adhesive joint. The sensor is a comb structure to measure the impedance of the adhesive over frequency. The structures are realized with microtechnologies, therefore they are ultra thin and flexible. Due to the progression of the impedance over time it is possible to draw conclusions about the curing process. With the presented sensor the curing of an adhesive can be measured.

L27 Wall effects on gas flow in large, alkyl-functionalized mesopores

Benjamin Besser, FB4, Advanced Ceramics

The gas permeation properties of mesoporous membranes with 20nm pore size are influenced by an altered surface chemistry. An alkyl-functionalization leads to a reduced permeability of an order of magnitude and an increased selectivity towards CO_2 which increases with temperature up to 30%. Both, the reduced permeability and the increased selectivity are not in agreement with the Knudsen theory, which is considered to be applicable.

Poster Session 2

15:00 Poster session and coffee break

Notes …

Novel aqueous zinc-ion battery based on copper hexacyanoferrate for grid energy storage

Fabio La Mantia, FB4, Energiespeicher- und Energiewandlersysteme

The need of economically feasible large-scale energy storage systems is the key factor in increasing the installation in the grid of volatile power sources, such as wind and solar. Aqueous metal ion batteries have shown to be a possible technology, which has the characteristics necessary for this application, such as safety, cost, and power output. Here, we report a new zinc-ion battery based on copper hexacyanoferrrate and Zn foil in 20 mM $ZnSO_4$, a nontoxic and noncorrosive electrolyte with pH 6. The voltage of this novel battery system is as high as 1.73 V. Cycled at a specific current of 60 mA g^{-1} (1C), the battery has shown a specific charge of 54 mAh g^{-1}, retention of specific charge after 100 cycles equal to 96.3%, and coulombic efficiency close to 99% during all the cycling. When the cycling rate was increased to 150, 300, and 600 mA g^{-1}, the reversible specific charge decreased to 96.1, 90 and 81 % of the initial value, respectively. The behavior of the system was reversible, upon decreasing the specific current back to 60 mA g^{-1}. This suggests that the aqueous rechargeable CuHCF-Zn battery can be charged and discharged very rapidly without affecting the stability of the electrodes. This property is ideal for its use in grid, where fast changes in the regime are required. The average specific power of the cell during discharge at 60 mA g^{-1} was 52.5 W kg^{-1} on the basis of the electrode active materials, and a specific power of 477 W kg^{-1} at 10C was reached.

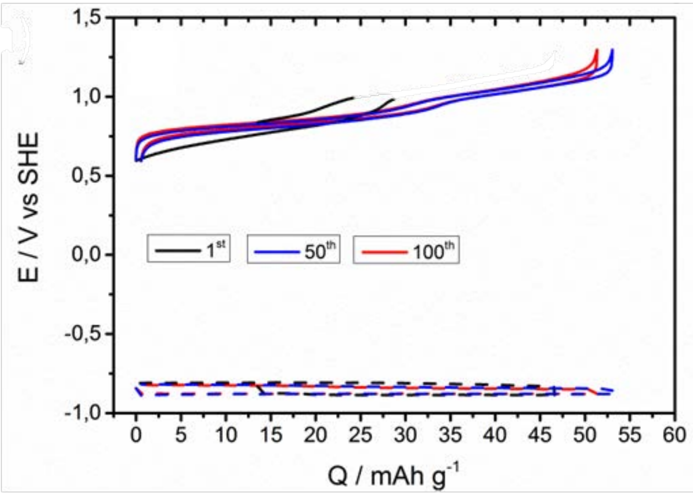


Figure: *Charge-discharge profile at different cycles of CuHCF (solid line), Zn film (dashed line)*

Social Event

17:00	**End of workshop**

move to Schwarzlichthof

18:00	**Dinner and blacklight minigolf**

Schwarzlichthof Bremen

???	**open end**

How to get there?

Schwarzlichthof, Cuxhavener Strasse 7

By car:
follow Hochschulring (B6) and Osterfeuerberger Ring to Waller Ring, turn left to Nordstrasse until Cuxhavener Str.

By bus/tram:
Linie 28 (Uni Central to Bremen Waller Ring)
17:05 (every 15 minutes)
5 minutes walk (turn left to Waller Stieg until Cuxhavener Str.)

Organizing committee

Hanna Lührs, MAPEX
Susan Köppen, FB4
Michael Fischer, FB5

2nd MAPEX Young Scientist Workshop
List of Participants

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2. **Aminian, Alieh**, FB4
3. **Bardenhagen, Ingo**, FB4, Innovative Sensor and Functional Materials
4. **Baric, Valentin**, FB4, IWT
5. **Besser, Benjamin**, FB4, Advanced Ceramics
6. **Bloem, Arne**, FB4, bime
7. **Braud, Nicolas**, FB1, Institute of Solid State Physics
8. **Brüggemann, Dorothea**, FB1
9. **Bunge, Frank**, FB1, IMSAS
10. **Delle Piane, Massimo**, FB4, BCCMS
11. **Dirks, Jan-Henning**, Hochschule Bremen - Biomimetics
12. **Dittmar, Anna**, FB4
13. **Dumstorff, Gerrit**, FB1, IMSAS
14. **Ebrahimi, Alireza**, FB4, Werkstoffmechanik - Computational Material Modeling
15. **Ewert, Moritz**, FB1, Institute of Solid State Physics
16. **Fischer, Simon**, FB1, Institute of Solid State Physics
17. **Fischer, Michael**, FB5, Crystallography
18. **Flosky, Hendrik**, BIAS
19. **Foremny, Eike**, FB4
20. **Franke, Jan**, FB4, BIK - Institut für integrierte Produktentwicklung
21. **Glenneberg, Jens**, FB4
22. **Haag, Katharina**, Hochschule Bremen - Biomimetics
23. **Herrmann, Marius**, FB4, bime
24. **Hildebrand, Nils**, FB4, BCCMS
25. **Hoffmann, Ron**, FB2, IFAM
26. **Hollermann, Gesa**, FB4, Advanced Ceramics
27. **Hölzen, Hauke**, FB5
28. **Hoog Antink, Marieke**, FB4, Advanced Ceramics
29. **Hoppe, Martin**, FB1, Institute of Solid State Physics
30. **Horosko, Alexej**, FB4

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34. **Kerlé, Daniela**, FB4
35. **Klein, Thorsten**, FB1, BIAS
36. **Köppen, Susan**, FB4, BCCMS
37. **Krisponeit, Jon-Olaf**, FB1, Institute of Solid State Physics
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42. **Langstädtler, Lasse**, FB4, bime
43. **Laube, Jens**, FB4, BCCMS
44. **Lehmhus, Dirk**, FB4
45. **Lid, Steffen**, FB4, Hybrid Materials Interfaces Group
46. **Liu, Yang**, FB4, bime
47. **Lorenz, Jonathan**, FB4
48. **Lucklum, Frieder**, FB1, IMSAS
49. **Lührs, Hanna**, MAPEX
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54. **Schenck, Christian**, FB4
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56. **Struß, Adrian**, FB4, Bremer Institut für Strukturmechanik und Produktionsanlagen
57. **van den Driesche, Sander**, FB1, IMSAS
58. **Weber, Lena**, FB1

2nd MAPEX Young Scientist Workshop

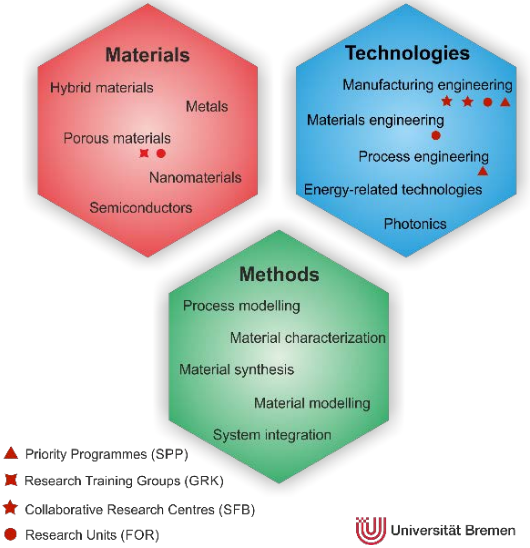
The workshop aims to bring together young scientists (PhD and MSc candidates, post-docs) from the University of Bremen and surrounding institutions who would like to find out more about ongoing research activities in the field of materials science. The workshop will comprise one plenary talk by Prof. Fabio La Mantia and three keynote presentations by MAPEX early career investigators who will highlight different aspects of the MAPEX research landscape. The participating PhD and MSc students will have the opportunity to present their research in poster presentations, accompanied by short oral "lightning presentations". The poster sessions will provide plenty of time for discussions in order to connect participants from different areas of MAPEX. After a day full of scientific insights, the participants will embark on a trip to the blacklight minigolf course, where the focus will be on social rather than scientific interactions. The workshop will be a platform for you 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.

MAPEX

A new form of Research Governance with the aim to:

- establish and maintain a network of competencies in the fields of materials science, materials technology,and materials processing
- increase the visibility of the Research Landscape
- apply for and participate in third-party funding programs
- promote cooperative research activities of junior scientists
- support an interdisciplinary doctoral education
- cooperatively acquire and share scientific equipment



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