

# SCIENCE & PROJECTS

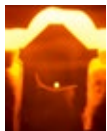
## Recently funded large-scale projects

### II COLLABORATIVE RESEARCH CENTER

#### Collaborative Research Center SFB 1232 "Von farbigen Zuständen zu evolutionären Konstruktionswerkstoffen"

The MAPEX Principal Investigator Prof. Lutz Mädler (IWT) initiated and successfully applied for the collaborative research center "Farbige Zustände" which will start on July 1st 2016. The consortium includes 10 MAPEX members from Institut für Werkstofftechnik (IWT), Bremer Institut für Strukturmechanik und Produktionsanlagen (bime), and Bremer Institut für Angewandte Strahltechnik (BIAS). Further members are from the Center for Industrial Mathematics (ZeTeM), the Center for Environmental Research and Sustainable Technology (UFT), the Group of Computer Architecture (AGRA) and the Max-Planck-Institut für Eisenforschung (Düsseldorf).

The initiative „Farbige Zustände“ (engl.: "Colored States") aims at the exploration of a novel experimental method for the development of evolutionary metallic structural materials. The overall goal is the efficient and focused identification of compositions and process chains, which result in a specific performance profile of the structural material. Conventional materials developments are based on costly experimental investigations of chemical, mechanical, or technological material properties. Such expensive requirements reduce the number of possible experiments, so that mostly predictive (or intuitive) approaches are employed. As a result, potentials of non-intuitive parameter choices are not taken into account. Combining new processes for primary shaping, micro structure formation ("coloration") and characterization of microscopic material samples, sample logistics as well as mathematical and computer science based methods for the analyses of large amounts of data, this research initiative develops of a novel high throughput method.



*Two of the novel processes developed in the collaborative research center SFB 1232: single droplet generation for micro-sample synthesis (left); micro-machining of single particles (right).*





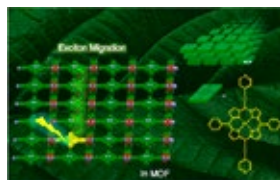
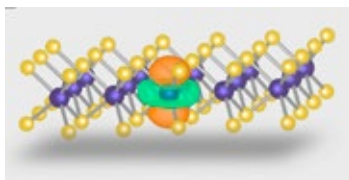
### New DGF Research Training Group (RTG) in Computational Materials Science

Within the GRK 2247, coordinated by the two MAPEX members Thomas Frauenheim and Tim Wehling, interdisciplinary research projects for twelve PhD students and two postdoctoral researchers in the field of Computational Materials Science will be funded at the University of Bremen, the Jacob University Bremen, the Carl von Ossietzky University of Oldenburg and the Max-Planck Institute for the Structure and Dynamics of Matter in Hamburg.

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In the last two decades, theoretical physicists and chemists have learned how to predict the outcome of chemical reactions with very high precision. They are able to numerically solve fundamental quantum mechanical problems with the help of large supercomputers. However, these solutions are based on approximations that are not valid for a wide range of important physical and chemical effects, such as photovoltaics or metal corrosion. Especially challenging is the description of materials with properties dictated by the strong correlation between their electrons (many-body effects). Also difficult to predict is the exchange of electrons across materials interfaces caused by interaction with light, which is for instance the basis of photocatalysis.

Although advanced approaches for the individual problems exist, the comprehensive understanding and the prediction of electronic properties for the rational design of advanced materials requires the development of modelling methods across the boundaries of traditionally separated subfields. The GRK 2247 has the mission of unifying different quantum mechanical materials modelling approaches and apply them to the two emerging topics of two-dimensional materials and metal-oxide interfaces. The unique interdisciplinary concept for the education of young scientists is embedded in a consortium in which the four research institutions mentioned above join their efforts in a brilliant example of Hanseatic cooperation.



*Materials modeling methods at different levels of accuracy will be applied to two-dimensional materials (left) and functionalized oxide materials (right).*



## II RTG 2224: $\pi^3$ : PARAMETER IDENTIFICATION - ANALYSIS, ALGORITHMS, IMPLEMENTATIONS

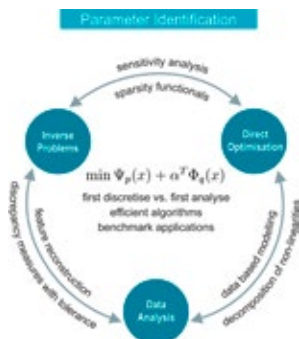


### New DGF Research Training Group (RTG) in Industrial Mathematics

Mathematics is a universal language, which allows to extract, model and analyze complex structures of different nature in a common abstract setting. Applied mathematicians go one step further and aim at relating the theoretical findings to real life applications. The newly funded RTG 2224, whose spokesperson is MAPEX member Peter Maass, combines mathematicians of the Center for industrial mathematics with mathematicians from computational topology, statistics and analysis.

The guiding principle of RTG 2224 is parameter identification, which relates to retrieving biological, physical, or technical parameters from measured data, or to determine system parameters for the optimization and controlling of complex processes. Accordingly, parameter identification is at the core of multiple applications in all fields of natural sciences, engineering, life sciences, and industrial applications. The demand for tackling even more complex models in terms of non-linearity, sensitivity, coupling of systems, or for including specific expert information as side constraints, provides numerous challenges in mathematical modelling as well as for designing, analyzing, and implementing appropriate algorithms.

Under the guidance of experienced scientists from the University of Bremen 24 PhD students (12 PhD positions funded by DFG) and several PostDocs will focus on the identification of deterministic high-dimensional and non-linear parameters for benchmark applications such as mass spectrometric imaging, optimization of automotive carburetor systems or optical analysis of fibre structures.



## II CHEMICAL IMAGING AND IN-SITU STUDIES OF 3D MICROSTRUCTURE EVOLUTION

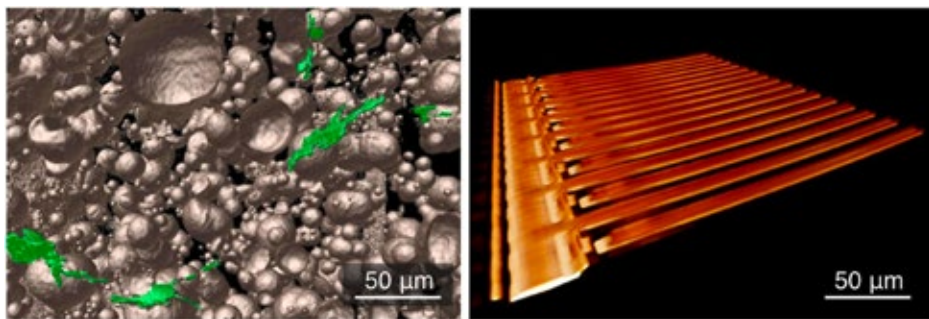
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### DFG major equipment funding: 2.4 Mio Euro for high-end X-ray Microscope

As one of six German institutions and less than one year after the official kick-off, MAPEX was successful within the major equipment call of the DFG for X-ray microscopes. Coordinated by the MAPEX speaker Lucio Colombi Ciacchi, eleven Professors of the University of Bremen were involved in the proposal *"In-situ studies of 3D microstructure evolution and spectroscopic imaging during processing and manufacturing of advanced materials"*. Thanks to recent advances of X-Ray Microscopy (XRM) and on-going efforts into fabricating spectroscopic detectors that allow a simultaneous detection of 3D microstructural maps and 3D chemical imaging, we will be able to open wholly new ways for a knowledge-based, concurrent development of materials and processes. Furthermore, a set of accessories will be developed to place samples under thermal, mechanical, or chemical load in the XRM sample chamber to enable in-situ studies of the effects of such loads on the materials microstructure and composition.

After the installation of the new equipment (Zeiss Xradia 520 Versa) in late 2016, routine measurements and service orders will be possible from early 2017. A detailed description of the new instrument will be published in one of the next newsletters.

"This success once more demonstrates the strength and relevance of the intense cooperation of the University with the external research institutions that makes Bremen an excellent science location", remarks Andreas Breiter, vice rector for research and young academics, University of Bremen.



*Examples of XRM imaging of a steel sample (left) produced by selective laser melting after bending test including micro-fractures (colored in green) and of portion of a microsensor element (right) showing work-hardened zones at the electrode base.*