

# **Scientific Project Portfolio**

**Expertise and Ideas for Cooperations** 





#### We are Young Investigators

The independent Junior Research Group Leaders and Junior Professors of the Karlsruhe Institute of Technology (KIT) are organized in the Young Investigator Network (YIN). Members have already proven their high potential in official selection procedures e.g. for a Emmy Noether-Program (DFG) or a Starting Independent Research Grant of the European Research Council (ERC). Furthermore, long lists of scientific publications give evidence of their outstanding research results.

#### We cooperate

Working together with industry, YIN identifies potential innovations and advances the economic application of scientific results from their young investigator groups. We look to industry cooperation to support and guide the transfer of technologies. As leaders of young investigator groups from diverse disciplines, we are interested in shaping the future of industry and society by tying in our competences with successful cooperative project and providing novel technologies.

#### We are connected

Since its foundation in 2008, the YIN developed into a strong democratic platform for peers, counting roughly 50 to 60 members throughout the years. The members meet regularly and develop solutions for common challenges by jointly organizing their interests, sharing their interdisciplinary knowledge, and diverse experiences. YIN, furthermore, maintains contacts to the executive board at KIT as well as to high representatives from science, politics and industry.



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## **Sustainable Software Systems Engineering**

#### Special expertise

Sustainability
Software engineering
Requirements engineering
Business Process engineering



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#### Abstract

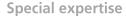
I am working on sustainability aware software system engineering. Sustainability has often been equated with environmental issues, but it is increasingly clear that it requires simultaneous consideration of environmental resources, societal and individual well-being, economic prosperity, and long-term viability of technical infrastructure. But, in traditional engineering processes these effects are usually not made explicit. This makes it hard to assess the long-term and cumulative impacts of a software system. So, solutions are needed to help the software engineers to understand and assess the systemic effects of decisions taken in requirements engineering and systems development under uncertainty.

Currently, I am focusing on requirements as the key leverage point for developing sustainable software-intensive systems. The sustainability challenge, however, cannot be tackled by technology alone, calling for a holistic approach. Business Process Management offers a comprehensive approach for designing, implementing, executing and monitoring business processes, with the support of technology. Thus, I am working on the conceptualization and integration of sustainability in business process management.

http://www.aifb.kit.edu/web/Stefanie Betz



#### **Carbon Nanotube Solar Cells and Sensors**



Carbon nanotubes Organic electronics Solar cells Energy



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#### Abstract

In our work we capitalize on the unique optical and electronic properties of carbon nanotubes for energy and organic electronic applications. We are interested in the purification and sorting of carbon nanotubes and have the ability to prepare large quantities of electronically or chirality pure single and double walled carbon nanotubes.

This allows us to develop strategies to control the order and orientation of this 1 D nano-material on the macro and nano-scale and for its combination with other organic active materials.

To this end we have developed carbon nanotube inks for the formation of thin films, from which new all carbon solar cells, photosensitive elements and sensing devices can be built.

http://www.int.kit.edu/flavel.php



# Materials tribology



Materials science Tribological systems Microstructure analysis and electron microscopy Bioinspiration and biomimetics



Contact
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#### Abstract

My group focuses on materials science aspects of materials under a tribological load. Our main research topics are:

- The elementary mechanisms for microstructural changes
- Size effects
- Contact mechanics
- Reciprocating contacts and dead center effects
- Bio-inspired materials and structures

In order to be able to answer these questions:

- We develop and build our own equipment and instrumentation, e.g. an extremely high resolution in situ reciprocating tribometer
- Make use of ultra-high resolution electron and ion microscopy, including 3D reconstruction techniques
- Morphologically texture surfaces by means of laser radiation
- Employ modern x-ray techniques, including from synchrotron sources
- Collaborate with scientists on an international basis



#### BNT-BT as the future lead-free functional material for PTCR



Piezoceramics
Ceramic processing
Diffraction
Defect chemistry



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#### Abstract

PTCR (positive temperature coefficient of resistance) and electrocaloric materials play an important role for energy efficient heating and cooling applications, especially in electric vehicles. The potential of the electrocaloric effect (ECE) for cooling applications to date is not technically exploited. Actuators play a crucial role in reducing the fuel consumption in combustion engines. Despite extensive studies and governmental regulations all over the world, most of the materials for PTCR, actuator and sensor devices are still based on lead containing ceramics which are toxic and harmful to the human body and the environment. During processing, highly volatile lead-oxide is released and with increasing demand sustainable disposal becomes a significant issue. Amongst the promising systems for novel sustainable lead-free functional materials, barium titanate (BT) based and bismuth sodium titanate based ceramics (BNT) emerged exhibiting significantly improved properties through doping.

The aims of this project are to understand the influence of doping on the PTCR, ECE and piezoelectric properties of BT-based lead free alternative functional materials and to derive guidelines for the development and implementation of this new class of materials. The key focus will be to define the defect chemistry as well as transport and strain mechanisms.

http://www.iam.kit.edu/kwt/399 2877.php



# Green Mobility: Tailored high-performance composites for weight-optimized automotive structures

#### **Special expertise**

Simulation of composites
Draping simulation of textiles
Modelling of manufacturing effects
Process and structural optimization of composites



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#### Abstract

Development of high-performance composite structures is very cost intensive, mainly caused by numerous manual iteration steps which are still necessary to find the optimal design in conjunction with the optimal process control. Additionally, composite components are often highly oversized due to the discrepancy between the real material behavior, largely influenced by the processing history, and the idealized models used in structural simulation. During the draping process, the fiber architecture is considerably modified, resulting in varying fiber orientations and local draping effects. These changes in material characteristics influence the mechanical performance and need to be considered for sizing and virtual validation of composite structures.

The Vector Stiftungs-Young Investigator Group "Green Mobility" pursues these objectives by developing efficient draping and structural simulation models, by holistically combining both simulation domains via data transfer, and by providing general solutions to determine optimized draping strategies in conjunction with optimized structural design.

https://www.fast.kit.edu/lbt/4590\_yig.php



# Capillary suspensions for versatile, cost efficient and ecofriendly material design

#### **Special expertise**

Suspensions and dispersions Porous materials Coatings and films Rheology



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#### Abstract

When a small amount of a second immiscible liquid is added to the continuous phase of a suspension, the rheological properties of the mixture are dramatically altered from a fluid-like to a gel-like state or weakly elastic to strongly elastic state, increasing the yield stress and viscosity by several orders of magnitude. This transition is attributed to the capillary forces of the two fluids on the solid particles.

The CapS research group studies the material properties of these suspensions as well as applications where this capillary suspension concept can be utilized. We investigate the properties of the induced particle network using microscopy techniques, where the network can be imaged in 3D and directly manipulated. Changes to the network are then connected to changes in the macroscopic material properties as measured using rheological techniques. This adjustable material response can then be used for the intelligent design of crack-free films, highly porous materials and environmentally friendly substitutes.

https://www.mvm.kit.edu/english/3757.php



## **Architecture-driven Requirements Engineering**



Software architecture Requirements engineering Software engineering



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#### Abstract

The research group is concerned with the evaluation of software architectures for the systematic support of decisions related to architecture design and requirements.

The motivation of our research is, that quality attributes of software, such as performance, reliability, and maintainability, are crucial for the success of software-intensive systems. In particular, decisions about the software architecture impact whether sufficient quality can be achieved. Correcting wrong architecture decisions can lead to high costs. Furthermore, errors in elicitation and analysis of quality requirements can result in wrong architecture decisions and unsuited architectures. Such errors consequently are a risk for the success of a software-intensive system.

The aim of our research group is to enable an iterative approach to architecture design and requirements engineering to minimize the risk of wrong architecture decisions and errors in requirements. The design space of software architectures shall be semi-automatically explored and be evaluated according to relevant quality attributes. Based on this evaluation, feedback for the specification of quality requirements can be provided. In particular, this approach shall clarify for architects and stakeholders which degree of quality can be achieved at which costs.

http://are.ipd.kit.edu/



**Young Investigator Group** 

# **Microarray Technology and Application**



Surface functionalization and microstructuring Combinatorial chemistry, high throughput screening Infectious disease research, bioinformatics Optical laser processing



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#### Abstract

High-density arrays represent an attractive method for high-throughput identification of molecular interactions. They are essential to reduce the consumption of reagents required for assays and, thus, save rare or expensive samples. Our current research topics in microarray technology and application are: (1) Development of matrix-based combinatorial array technology (Physics, Engineering, Chemistry); (2) antibody profiling for infectious diseases (Biomedical research, Bioinformatics).

For comprehensive antibody serum readout, regarding e.g. the malaria parasites, we translate the genomic information from databases into sequences of overlapping peptides. Depending on the sequence of their 20 different amino acid building blocks, peptides are a major class of antibody binders, which qualifies them to be used as diagnostic biomarkers or therapeutics. Therefore, a large set of different peptides has to be synthesized and screened in order to find e.g. novel biomarkers. Today's peptide array market is still dominated by the over 20 year old SPOT synthesis, which provides only low spot densities achieving at most a few hundred spots per cm² if pre-synthesized peptides are spotted. We developed a novel method of peptide array synthesis, which combines the high spot densities achieved by light-controlled lithographic methods with the cost-efficiency of one-cycle-per-layer coupling in solid matrix material based synthesis.

http://www.yin.kit.edu/english/1103 1621.php



## **Theoretical Computer Science / Parallel Computing**



Big graph analytics
Parallel computing
Combinatorial optimization
Algorithm engineering



Contact
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#### Abstract

The research group Theoretical Informatics and Parallel Computing headed by Henning Meyerhenke works at the interface of algorithms, parallel computing, and applications in networked systems. We often follow the methodology of Algorithm Engineering. This means to iterate the design, analysis, implementation, and systematic experimental evaluation of algorithms, in particular graph algorithms.

Our focus is on algorithms that are suitable for large problems and that make use of the computational power of parallel systems. Three application areas are of main interest, algorithmic network analysis, combinatorial scientific computing, and applied combinatorial optimization.

http://parco.iti.kit.edu



#### Multiscale Models for Contact, Friction and Wear



Contact mechanics Adhesion Tribology

Atomic-scale simulation



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#### Abstract

Our research revolves around computer modeling of mechanical and chemical properties of material interfaces and their interaction with fluids and other solids. We have a particular focus on tribological phenomena (contact, adhesion, friction, lubrication, wear) that naturally occur at interfaces. Such processes are important in macro- and microsystems and their control is decisive for the lifetime of a device.

For example in miniaturized components that have a high surface to volume ratio, interfacial processes can entirely dominate mechanical behavior: At small scales, strength is determined by surface and not bulk defects, the flow of liquids through nanochannels can be controlled by surface topography and chemistry and surface forces such as adhesion and friction can overcome body forces and lead to stiction. Common to these phenomena is the interplay of local chemistry, long-ranged interaction (such as elasticity) and geometrical disorder (such as surface roughness). Models at atomic, mesoscopic and macroscopic scales are therefore required for their understanding.

https://www.yin.kit.edu/english/1103 1692.php



## **Superconducting Quantum Circuits**



# Contact Dr. Ioan Pop

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# **Special expertise**

Experimental quantum information Superconducting circuits Josephson junctions Cryogenic microelectronics

#### Abstract

Our research focuses on superconducting quantum circuits.

Josephson junctions have been proven to be reliable building blocks for superconducting quantum memories, high-speed processing units, amplifiers and detectors, operating in the microwave domain. In these types of electrical circuits, which can be manufactured using standard lithography, currents and voltages can exhibit quantum mechanical properties and can be controlled using microwave pulses. This makes them appealing for the study of fundamental quantum phenomena and the implementation of quantum information processing.

We are currently interested in the design and implementation of quantum circuits protected against decoherence.

https://www.phi.kit.edu/pop.php



## **Indirect Microfluidic Systems / Fluoropor**



Microfluidic systems
Additive manufacturing
Polymer synthesis (biopolymers, highly fluorinated polymers)
Biosensors



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#### Abstract

The focus of the research group is the development and application of microfluidic systems with a focus on the development of materials and manufacturing technology for creating such systems. Here, a focus is on usage of photopolymerizable materials, highly fluorinated polymers as well as ceramics and glass.

The group has extensive knowledge in chemical and physical surface functionalization and structuring as well as in the development of instruments for these techniques including rapid prototyping methods, 3D printing, as well as photolithography using custom-designed instruments.

http://www.neptunlab.org/



## **Adaptive Data Analytics**



Multimedia knowledge representations Explainable data analytics Machine learning, text mining, semantic technologies Knowledge graphs, semantic annotation



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#### Abstract

Information retrieval and machine learning approaches are running in the background of most of the applications we use in our daily digital life. The assistance they are providing is manifold, but relies only on a set of core information processing tasks, the most prominent ones being retrieval, classification, clustering and prediction of information. How media items with heterogeneous content representations, like text documents in different languages or text and images found online and on social media, can be processed jointly is the focus of this research group.

While the human brain has the ability to integrate disparate multi-sensory information into a coherent percept that benefits from all sensory information (hearing, seeing, etc.) current information processing technologies lack this ability. By combining machine learning with natural language processing and semantic technologies we fuse complementing information from all sources such as texts, images or knowledge graph. This enables cross-modal data analytics and provides a more holistic view than each modality separately.

http://www.aifb.kit.edu/web/Achim Rettinger/en



## Radio detection of high-energy cosmic rays



Digital antenna arrays
Time and amplitude calibration
Signal processing
Software frameworks for data analysis



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#### Abstract

Digital radio detection has become a promising technique for astroparticle physics. High-energy cosmic-rays initiate cascades of particles when they hit the atmosphere. These atmospheric particle cascades emit a radio pulse which can be detected by antennas on ground. With computing-intensive analysis techniques the signals of several antennas are processed and combined in order to extract information on the cosmic-ray particles.

For this purpose I participate in the largest antenna array for cosmic rays, which is in Argentina at the Pierre Auger Observatory. Moreover, I am responsible for coordinating a smaller antenna array in Siberia consisting of about 60 antennas on an area of one square kilometer. The work of my ground includes calibration methods for accurate timing as well as the development of software algorithms for improving analysis techniques of the radio measurments.

http://www.ikp.kit.edu/tunka-rex/



## **Dislocation-based Continuum Modeling of Crystal Plasticity**



Micromechanics and failure mechanisms Computation and simulation Dislocation based plasticity and homogenization Metallic composite materials



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#### Abstract

The research group focuses on the predictability of materials behavior and the reliability and safety of components with a special interest in metals. We use multi-scale material modelling and numerical simulation to combine small scale microstructural behavior and continuum mechanical analysis. Our goal is to enable insights into materials and structures in order to optimize the composition of materials as well as the shape of devices and investigate resource efficient systems. Considering the evolution of dislocations as fundamental physical effects causing plasticity as intentional or destructive deformation, we want to introduce a computational engineering tool which bridges the scales from micro to macro. Using physically based formulations, the evaluation of high risk areas in materials, e.g. interfaces in composites, and the investigation of fundamental failure mechanisms lead to new prospects in the assessment of materials and components.

Due to the multidisciplinarity of the topic, the group is composed of engineers, mathematicians, physicists, and material scientists, who bridge the issues from modelling physical phenomena, mathematical and numerical formulations, and efficient implementation to engineering applications



#### Computer assisted surgery



Computer vision for medical applications
Biomechanical registration
Intraoperative navigation and visualization
Sensor-based modelling and analysis of surgical workflows



Contact

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#### Abstract

New technological devices and technical procedures in surgery provide a huge amount of valuable patient data. However, to process the myriad information is an overwhelming challenge for physicians, especially in the operation room (OR).

The goal of my research is to develop and evaluate surgical assistance systems which optimize the therapy of the individual patient by turning the available data into useful information. Therefore, I am investigating the entire process chain along the surgical treatment path including pre-, intra- and postoperative patient information. Eligibility and success rates of surgeries can be significantly improved using personalized digital representations of the patient and enable the deployment of this data in the OR, e.g. by visualization of planning data or the prediction of complications.

To this end, we focus on multimodal analysis of intraoperative sensor data, biomechanical soft-tissue navigation as well as knowledge-based interpretation for context-aware assistance. This methods allows for the first time a context-aware assistance in the OR of the future, which acts as an automatic information filter, avoids information overflow, adapts to the current needs of the surgeon and therefore provides new man-machine interaction techniques.

http://his.anthropomatik.kit.edu/829.php



#### **Bio-inspired surfaces**



Polymeric nanocomposites
Carbon nanotubes
Polymeric nanofoams
Microfabrication



Contact

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#### Abstract

Functional adaptation through porous structures is well known in nature. In nature multi-leveled hierarchical porous networks do serve for certain catalytic, optical as well as mechanical functions. Such structures are made by direct organization of living cells and cannot be directly reproduced. We mimic the outstanding features of nature by modification of well-known polymers. The recent projects are Pomelo-inspired tuning of elasticity in polymeric foam by control of pore morphology and White-beetle-inspired ultrathin omnidirectional white films for enhanced reflection. For the both projects we create nanosized pores inside thermoplastic materials, such as PMMA or bio-degradable PLA by saturation in supercritical carbon dioxide

Similarly to hierarchical porous structure of the pomelo peel being a perfect example of energy dissipation we have created a polymeric foam with a gradient of pore size ranging from micro to nano range and investigated gradually changing elastic modulus of such a foam. Polymeric nanopores also serve as great scatterer of visible light similarly to Cyphochilus beetle. By optimizing the pore diameter and the filling fraction, we obtain very thin highly reflective films suitable for coating. The films demonstrate high thermal stability and can be further processed by moulding techniques.



# **Hierarchically Structured Biomaterials and Nanomembranes**

#### **Special expertise**

Microporous polymers Biointerfaces Material chemistry Interfacial synthesis



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#### Abstract

The goal of my research group is to develop novel biomaterials for applications in biotechnology and medicine. The materials are based on a new class of multifunctional network polymers, which are prepared via conversion of a crystalline template structure (metal-organic frameworks, MOF). This novel class of materials combines the advantages of MOF, namely their precise molecular structure and high compositional and structural variability, with the advantages of polymer gels, namely their stability in physiological media and their biocompatibility.

Such hierarchically structured materials, which are optimized at all length scales relevant for cellular activity could offer the necessary micro-environmental cues for cellular proliferation or differentiation in the right place and at the right time, which makes these biomaterials ideal candidates for applications in cell culture, tissue engineering, medical implants or wound dressing.

In additional projects we develop thin membranes of only a few nanometer thickness composed of different microporous polymers. Freestanding nanomembranes of the porous polymers with a hierarchical composition are prepared by a layer-by-layer (LbL) synthesis on sacrificial substrates. The membranes and thin films can find application in gas and liquid phase separation as well as in organic electronics.

https://www.ifg.kit.edu/2440.php



## Structure determination of the protein translocase Tat



membrane proteins protein expression and purification circular dichroism solid-state NMR



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#### **Abstract**

The "twin arginine translocase" (Tat) is a protein export machinery present in bacteria, archaea and plant thylakoids. In contrast to the ATP dependent Sec system, the Tat translocase transports large, folded proteins across the plasma membrane, driven only by the proton electrochemical gradient. In Bacillus subtilis the minimally active translocation complex consists only of the two essential transmembrane proteins TatA and TatC. The TatC protein recognizes the cargo via a "twin arginine" containing signal peptide, and TatA has been suggested to form the homooligomeric pore complex.

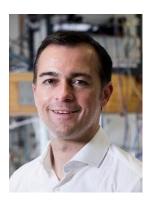
We have determined the membrane orientation of monomeric TatA by solid-state NMR and oriented circular dichroism spectroscopy. TatA consists of an unusually short  $\alpha$ -helical transmembrane segment (TMS), an amphiphilic  $\alpha$ -helix (APH) and a densely charged region (DCR) at the C terminus. Remarkably, the charges on the APH are perfectly complementary to those on the DCR. We thus proposed that the TatA pore assembles via these complementary charges, by forming ladders of intra- and intermolecular salt bridges. This so called "charge zipper" is a completely new folding motif in membrane proteins. Currently we are investigating the role of the unusually short transmembrane segment of TatA which seems to play an important role in the translocation process.



# Quantum manipulation and detection with superconducting qubits

# Special expertise

Quantum physics microwave circuits Hybrid solid state systems Quantum information processing



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#### Abstract

The ERC group experimentally interfaces ferromagnets with superconducting quantum circuits to study dynamics within the magnet. Superconducting qubits are ideal detectors due to their quantum limited back-action on the measured object and energy resolution. Spectroscopy and coherence measurements on the hybrid system are made in order to address fundamental aspects such as spin wave generation, detection, coherence, or wave propagation at ultra-low power.

Exploring spin wave dynamics by coupling to a superconducting qubit complements conventional measurement techniques based on photon, electron or neutron scattering methods, which require highly populated excitations. Magnetic material research is enhanced by new detection concepts such as quantum resolved spectroscopy and coherence measurements.

The project connects to and extends research objects of ground-breaking nature to open up new horizons for quantum computing, magnonics and spintronics. The group has extensive knowledge in linear and non-linear microwave circuits operated down to cryogenic temperatures, high frequency spectroscopy and time-domain electronics including measurement software, and quantum circuits for detection and computing.

http://www.phi.kit.edu/weides



#### **Manufacturing and Materials Technology**



Manufacturing processes
Planning and control of manufacturing processes
Surface engineering
Simulation of manufacturing processes



Contact

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#### Abstract

Product design is one of the core fields of engineering. As component properties are considerably influenced by manufacturing processes, there is an increasing need to take an interdisciplinary approach to this task, drawing on product design, production and materials technology. The design process must be geared towards these properties, which are influenced by individual machining steps throughout the whole process from raw materials or semi-finished products through to the finished product itself. Since these processes are highly developed, the challenges in this field mainly fall within the scope of production engineering research.

The main focus of Manufacturing and Materials Technology is the development and optimisation of processes and process chains in manufacturing and materials technology including production-related component properties. To cover all aspects, Manufacturing and Materials Technology is subdivided into fields of expertise Manufacturing Processes (Machining, Micro processing, Additive manufacturing, Heat and surface treatment), Process Planning an Control (Cooling and lubrication concepts, In-process control, Simulation of processes and -chains, Process-component-machine interaction) and Surface Engineering (Topography, Microstructure, Residual stresses, Work hardening, Fatique, Tribological stress).

http://www.wbk.kit.edu/english/26.php



# Overpotentials in High Temperature Proton Exchange Membrane Fuel Cells

#### **Special expertise**

Oxygen reduction reaction in electrolytes
Fuel cell membrane electrode assembly (MEA)
Characterization for proton exchange membrane fuel cells simulation
Catalysis



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#### Abstract

High-temperature proton exchange membrane fuel cells (HT-PEMFCs) based on phosphoric acid doped polybenzimidazole (H3PO4/PBI) membrane operate at elevated temperatures between 150 and 180 Degree Celsius. The HT-PEMFC stacks have much simpler water and thermal management than lower-temperature PEM fuel cells and can operate on reformat gas. These advantages make this type of fuel cells an interesting candidate for auxiliary and stationary power units. At this moment, however, no commercial HT-PEMFCs have been developed to meet the reliability and cost requirements.

The Young Investigator Group is exploring this field to understand the performance limiting mechanisms and find effective solutions. We address the issue of overpotentials in HT-PEMFC on three different levels: the cell level, the component level, and the microscopic or molecular level.

http://www.wbk.kit.edu/english/26.php