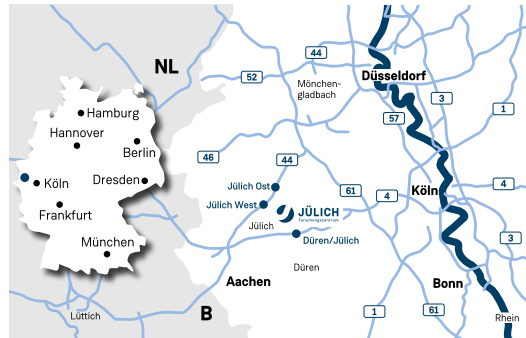


## HOW TO FIND US



## CONTACT

*Institute director:*

Prof. Dr. Olivier Guillon

Tel: +49 2461 61-5181

[o.guillon@fz-juelich.de](mailto:o.guillon@fz-juelich.de)

[www.fz-juelich.de/iek/iek-1](http://www.fz-juelich.de/iek/iek-1)

Forschungszentrum Jülich GmbH

Institute of Energy and Climate Research

Materials Synthesis and Processing (IEK-1)

52425 Jülich

Germany

## INSTITUTE OF ENERGY AND CLIMATE RESEARCH IEK-1: MATERIALS SYNTHESIS AND PROCESSING

Member of the Helmholtz Association

## EXCELLENCE IN MATERIALS SCIENCE AND ENGINEERING

Materials scientists, chemists, physicists, mechanical engineers and technical staff at IEK-1 focus on the development of inorganic materials (in particular functional ceramics) and multi-layered components for highly efficient future energy conversion and storage systems.



## RESEARCH AREAS

Bridging the gap between basic science and applications, our research encompasses:

### MATERIALS FOR HIGH-TEMPERATURE TECHNOLOGIES

**Prof. Dr. R. Vaßen**

Tel: +49 2461 61-6108

[r.vassen@fz-juelich.de](mailto:r.vassen@fz-juelich.de)

High-temperature materials, especially thermal and environmental barrier coatings for gas turbines deposited by thermal spraying (for power generation and aircraft engines)

### GAS SEPARATION MEMBRANES

**Prof. Dr. W. A. Meulenber**

Tel: +49 2461 61-6323

[w.a.meulenber@fz-juelich.de](mailto:w.a.meulenber@fz-juelich.de)

Gas separation membranes for oxygen and hydrogen production, including proof-of-concepts for gas supply and catalytic membrane reactors

### SOLID OXIDE CELLS

**Hon.-Prof. Dr. N. H. Menzler**

Tel: +49 2461 61-3059

[n.h.menzler@fz-juelich.de](mailto:n.h.menzler@fz-juelich.de)

Solid Oxide Cells (high-temperature and fuel cells), from materials development to cell manufacturing, performance increase and understanding of degradation.

### ELECTROCHEMICAL STORAGE

**Prof. Dr. D. Fattakhova-Rohlfing**

Tel: +49 2461 61-85051

[d.fattakhova@fz-juelich.de](mailto:d.fattakhova@fz-juelich.de)

Solid-state lithium and sodium batteries, from the development of electrolyte and active materials to the integration in full cells

### EXPERTISE

Our extensive expertise ranging from solid state chemistry and synthesis, powder-based and wet-chemical processing, sintering, to thin film and thermal spraying technologies has allowed for rapid adaptation to the emerging challenges in science, from battery research to ceramic matrix composites.

To fulfill our mission, 1,250 m<sup>2</sup> of excellently equipped lab surface, including two clean rooms and a new membrane center (15 Mio €, finished in 2016) are available. A unique research

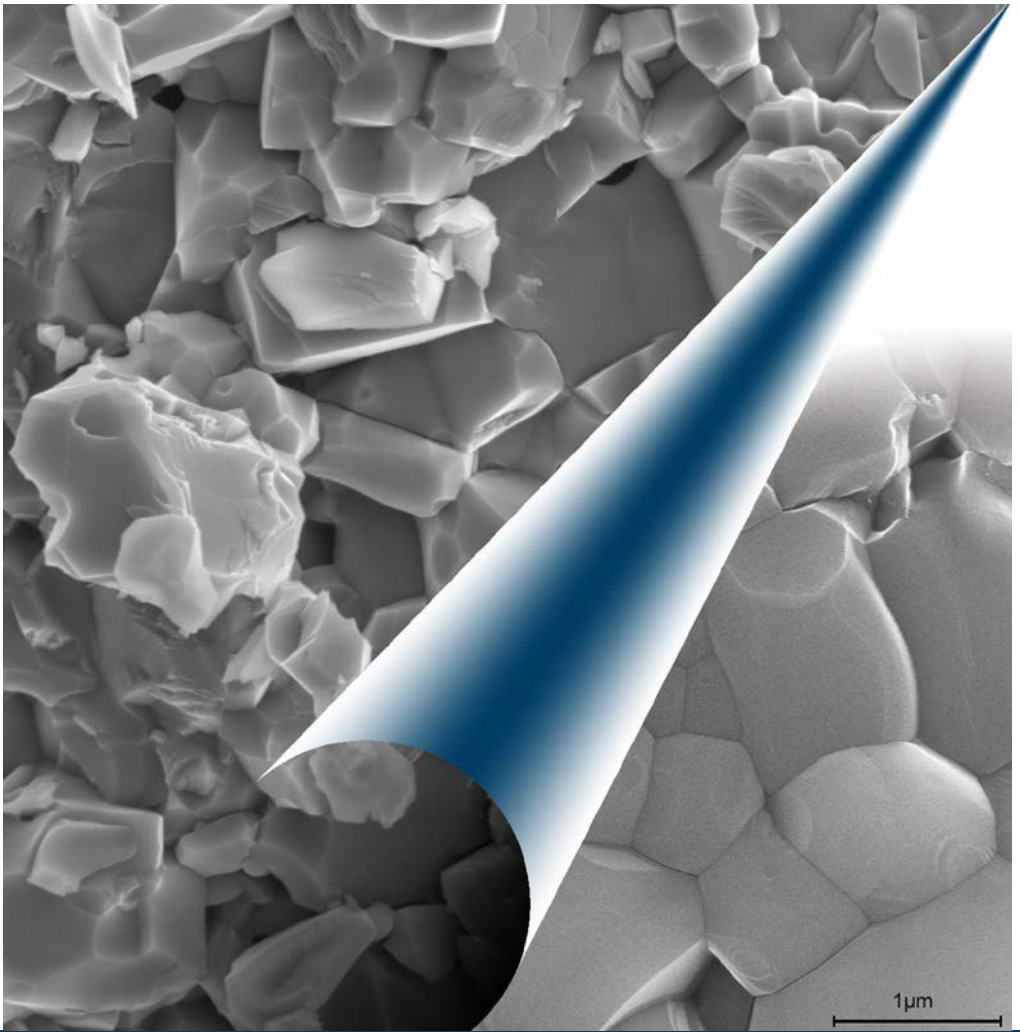
infrastructure offers more than 30 different materials synthesis routes, processing and coating technologies of inorganic materials such as ceramics and metals.

Experimental activities are complemented by modeling at the meso- and macroscopic levels Density Functional Theory (Monte Carlo simulations, Computational Fluid Dynamics, Finite Element Analysis), which allow a better understanding and prediction of materials and processes.

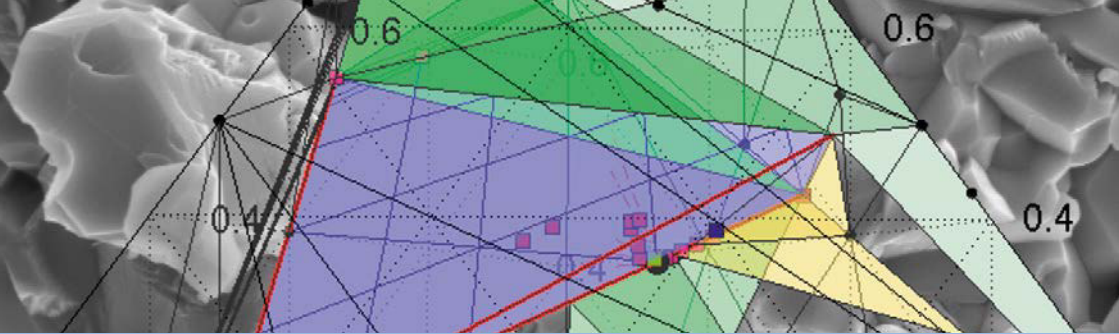
Our aim is to be at the forefront of the development of functional materials and production-relevant and scalable processing techniques, which facilitate technology transfer. A large part of our equipment meets industrial standards, supporting a strong collaboration with industry. Our extensive experience in project planning and management has resulted in several national and international coordinated consortia and research programs.

### PARTNERSHIP

We foster intense collaboration within our growing network of academic and industrial national and international partners. Furthermore, we established close strategic cooperations with neighboring universities (RWTH Aachen University, Ruhr Universität Bochum, Universität Duisburg-Essen as well as University of Twente, NL) in the frame of professorships, as well as with WWU Münster (through Helmholtz Institute Münster).



# MATERIALS DEVELOPMENT



## MATERIALS DEVELOPMENT

Functional materials and electroceramics – these are the keywords of our scientific research, either at high temperatures or at ambient conditions, either ionic conductors or electrocatalysts: more than 20 years of experience are the basis for further innovations.

### GENERAL SCOPE

The team „materials development“ is focused on the preparation of powders for ceramic and composite materials. From classic and novel synthesis methods to large-scale production, the powders are specially produced for use in electrochemical applications. The applicability of the materials is evaluated on the basis of chemical and physical properties initially investigated on generic ceramic specimens. Materials of interest are then processed to realistic components using conventional ceramic technologies and the materials' quality is optimized for the intended application.

### CURRENT DEVELOPMENTS

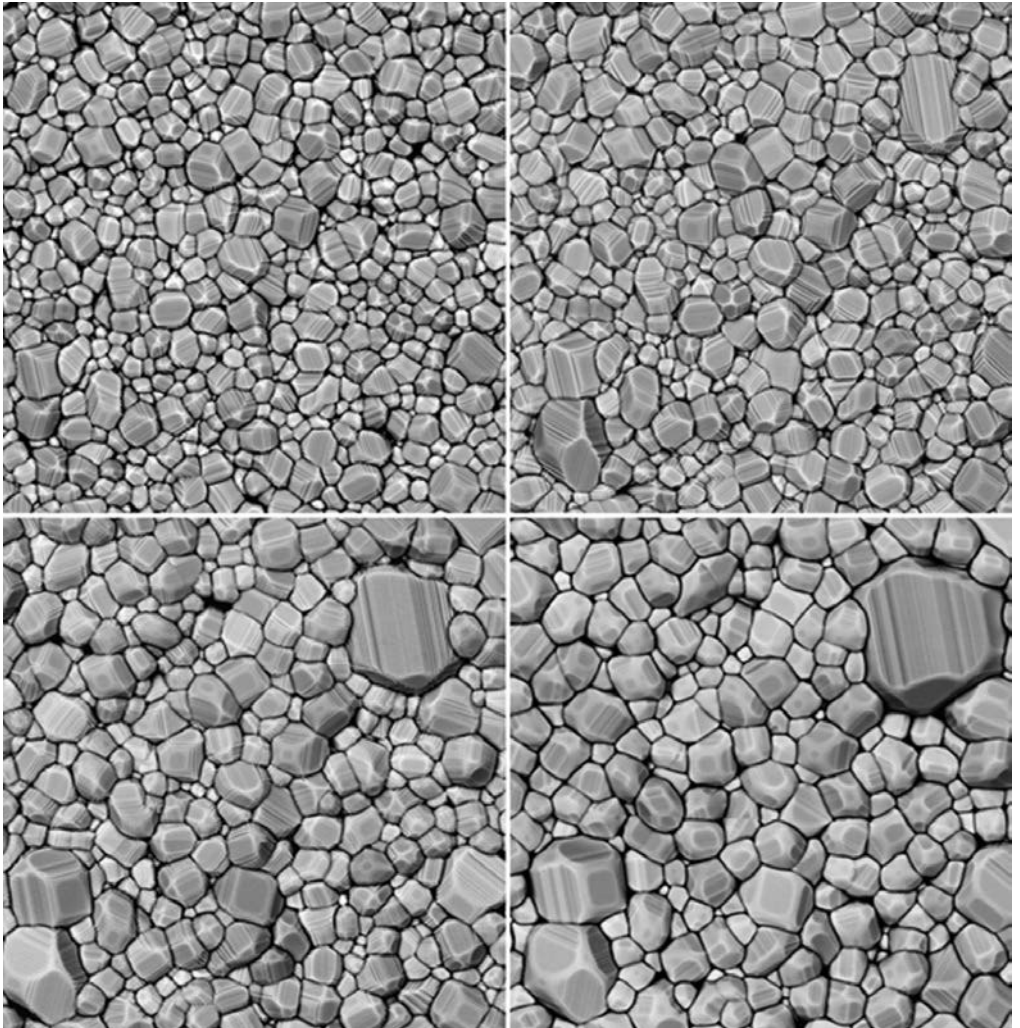
Triggered by the need for better energy storage systems for future energy supply, the team is working on new battery materials. Major effort is devoted to solid electrolytes with the aim to develop safe and large-scale solid state batteries for stationary applications and other electrochemical applications. The research includes low-cost and tailored synthesis methods and experienced processing aiming to produce dense ceramics as ion-selective membranes. Depending on the target size and application, the thickness of the membranes may be varied from 10  $\mu\text{m}$  to 1 mm using different fabrication technologies. Presently, the materials under investigation are NaSICON-type lithium- and sodium-ion-conductors.

Using our experience in electroceramics, the team also works on electrode materials, especially on cathodes for solid state batteries and on the interaction between solid electrolytes and cathode materials.

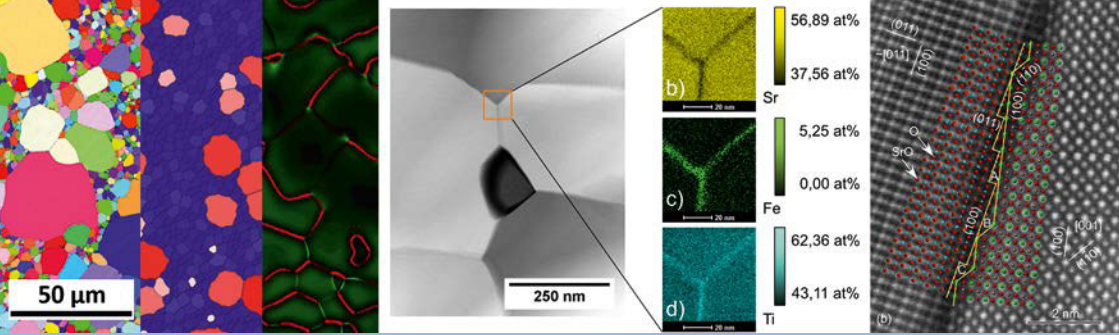
### CONTACT

Dr. Frank Tietz  
Tel: +49 2461 61-5007  
f.tietz@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# INTERFACES IN FUNCTIONAL CERAMICS



## INTERFACES IN FUNCTIONAL CERAMICS

### HOW TO TWEAK MATERIAL'S PROPERTIES FOR FUTURE ENERGY APPLICATIONS?

Interfaces play a key role in materials processing and microstructure evolution of ceramic materials and dominate many material's properties. In conducting ceramics, such interfaces involve space charge, which results in low grain boundary conductivity posing a significant roadblock for applications as electrolytes in SOFC or solid-state Li batteries.

### SPACE CHARGE AND SEGREGATION

Besides functional performance, segregated defects also dominate densification and grain boundary migration. The underlying physics are known since the 60s ('solute drag'). Tailoring microstructure evolution in functional ceramics for a given application needs a fundamental understanding of space charge and segregation from both a processing and properties perspective.

### GRAIN BOUNDARY ADSORPTION AND ITS INTERPLAY WITH FUNCTIONAL PROPERTIES

Grain boundary phases ('complexions') are pivotal for microstructure evolution and functional

properties. In LMO-LLTO half cells and similar systems for solid state batteries, nm-thick layers of amorphous grain boundary phases can result in enormous interfacial resistance rendering the solid-state battery unusable. Accordingly, a careful control of grain boundary phases is needed for optimal performance.

### ATOMISTIC GRAIN BOUNDARY STRUCTURE

On atomistic scale, the motion of grain boundaries is believed to base on the movement of steps and dislocations ('disconnections'). This mechanism is overlaid by other effects as space charge and solute drag, which couple back into functional properties and performance.

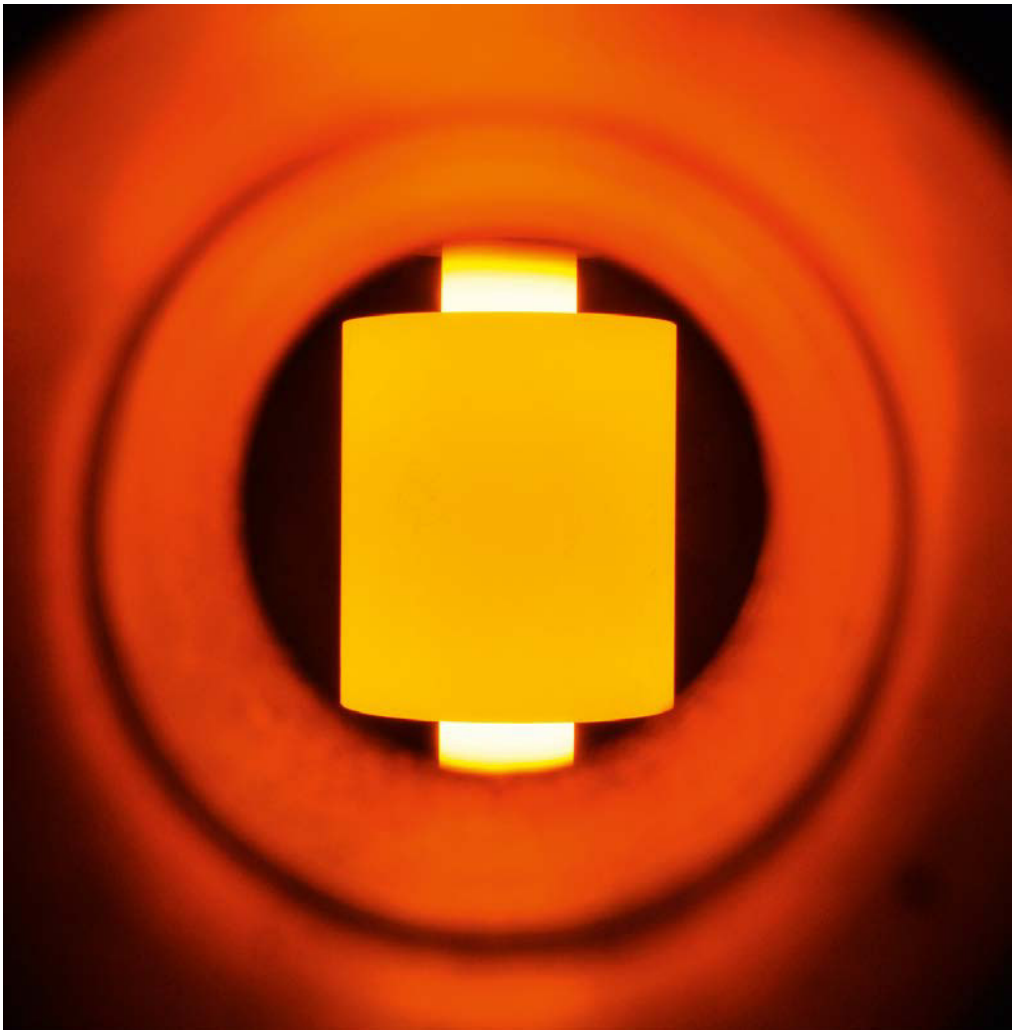
### SIMULATION OF MICROSTRUCTURE EVOLUTION

To obtain full microstructural control, digital twins of microstructure evolution and interfacial properties are needed, e.g., using a multi-physical phase field model for microstructure evolution. This model can also be used to predict functional properties.

### CONTACT

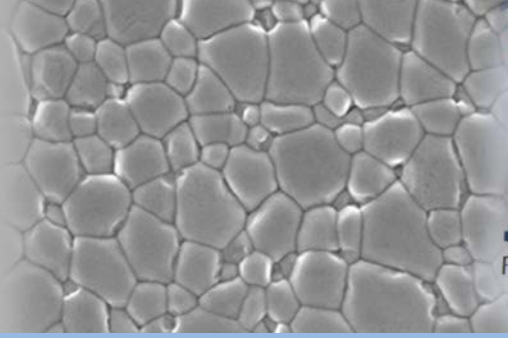
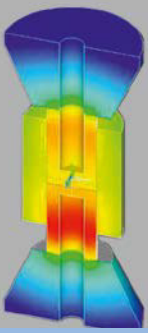
Dr.-Ing. Wolfgang Rheinheimer  
Tel: +49 2461 61-4382  
w.rheinheimer@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# POWDER-BASED PROCESSING AND SINTERING

Member of the Helmholtz Association



## POWDER-BASED PROCESSING AND SINTERING

The team “Particle-based processing and sintering” provides specific net-shaping and sintering technologies, which can be applied for metallic and ceramic powders. The equipment is comprised of technologies for net-shaping powders, as well as specific sintering technologies, which enable superpositioning of pressure and/or electric field, aiming at full densification of the ceramic.

### NET-SHAPING OF CERAMIC AND METALLIC POWDERS

The team deals with the net-shaping of metallic or ceramic powders by powder compaction, dip coating, tape casting or powder injection molding. A specific expertise exists in the processing of parts with well-defined porosities up to 80 Vol. %, which can be used e.g. as heat exchangers, current collectors, electrodes or metallic supports of electrochemical devices like fuel cells or gas separation membranes. Furthermore, we are able to manufacture metal-ceramic composites with layered structures and tailored interfaces.

### SINTERING UNDER PRESSURE AND/OR ELECTRICAL FIELD

Different sintering techniques are available to densify a wide range of ceramic and metallic powders (yttria, ceria, tungsten, titanium, etc.) up to the theoretical density. A hot press (HP) with a  $\text{MoSi}_2$  heating element enables sintering at temperatures up to 1600°C under vacuum, air and argon up to a maximum load of 100 kN.

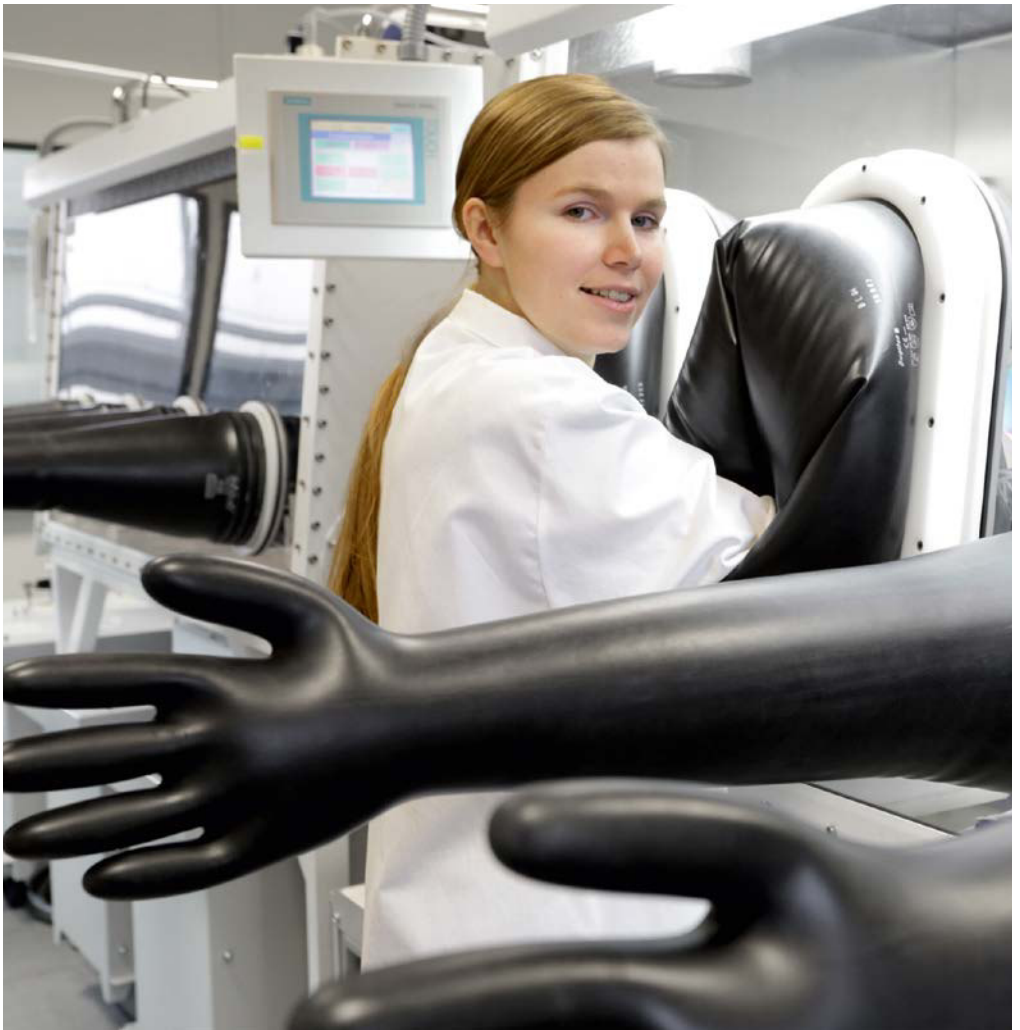
Three field-assisted sintering/spark plasma sintering (FAST/SPS) devices enable rapid densification of ceramic, metal or composite powders. Here, temperatures up to 2,200°C and pressures up to 100 MPa can be achieved with graphite tools. Higher pressures up to 400 MPa are possible with alternative tool materials. Another mode of operation is flash sintering with AC and DC voltages up to 1000 V accompanied by external heating via induction coil or  $\text{MoSi}_2$  heating element. A custom made sinter forging device equipped with programmable power source, electromechanical testing system and optical laser scanners enables in-situ measurement of sintering parameters like viscosity, sintering stress and viscous Poisson's ratio under electric field.

### CONTACT

PD Dr. Martin Bram  
Tel: +49 2461 61-6858  
m.bram@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany





## THIN FILM TECHNOLOGIES



## GAS PHASE AND LIQUID PRECURSOR-BASED THIN FILMS

Thin-film technology enables the mass production of highly complex systems. The development of efficient and thus economically viable production methods is an important aspect for all kinds of energy converters and storage devices. This is why IEK-1 relies on physical and chemical vapor deposition (PVD/CVD), atomic layer deposition (ALD) and coating technologies based on liquid precursors and inks.

### PHYSICAL VAPOR DEPOSITION

This technology is particularly suitable for dense layers on outer (“visible”) surfaces. IEK-1’s expertise is thermal and electron beam evaporation, pulsed laser deposition and magnetron sputtering (direct current, middle frequency, radio frequency, bi-polar or High Power Impulse Magnetron Sputtering). It is possible to deposit metals, as well as glasses or ceramics (for example oxides or nitrides).

### CHEMICAL VAPOR DEPOSITION

IEK-1 uses atomic layer deposition (ALD) for conformal coatings on inner surfaces of porous

materials. Single atomic layers are built up in succession to achieve dense layers of a few nanometers thickness. Relatively low coating temperatures (100–300 °C) can be achieved by using metal-organic precursors.

### LIQUID PRECURSOR-BASED FILMS

Wet-chemical coating methods are based on emulsions, sols or solutions which are coated on substrates. Subsequent heat treatment leads to dense layers. Spin coating, dip coating and inkjet printing in a cleanroom environment are used to apply the liquids.

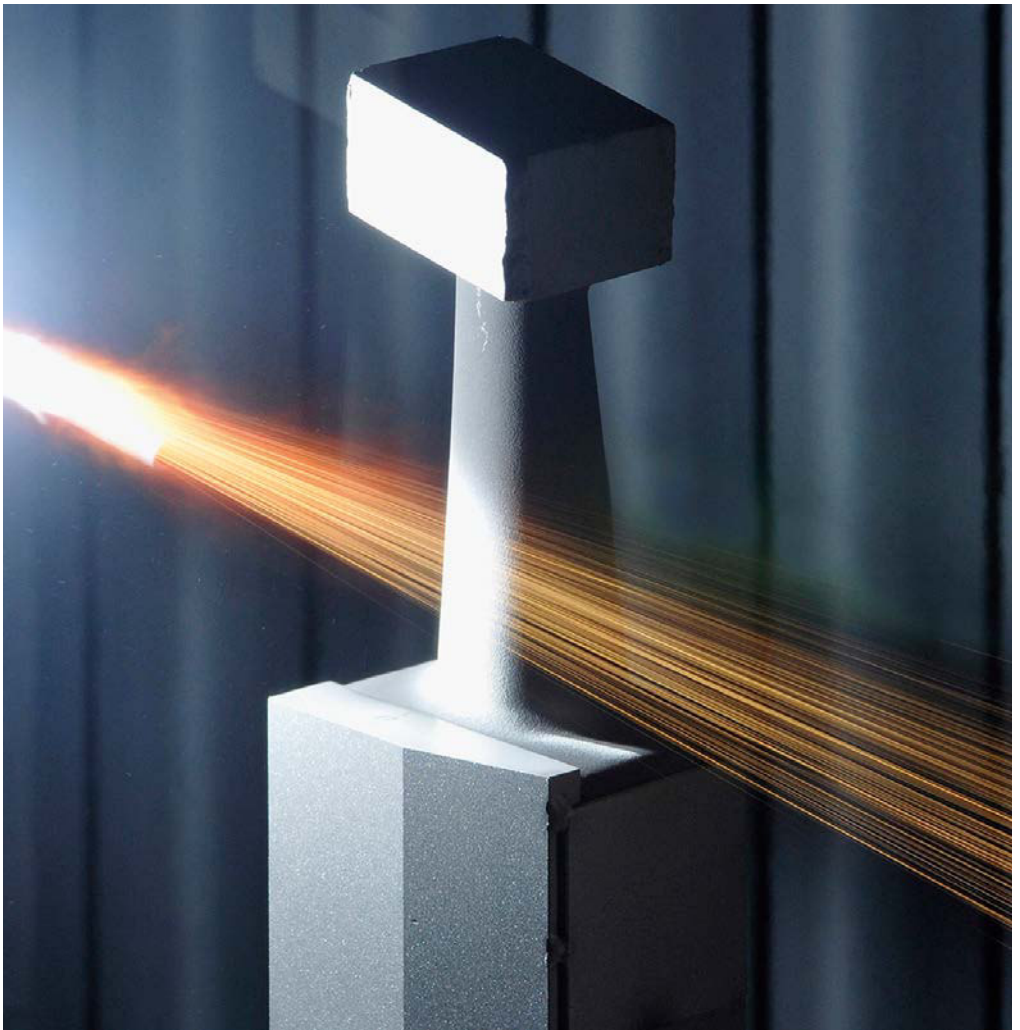
### APPLICATIONS

Thin-film technologies at IEK-1 lead to outstanding performance improvements of energy converters and storage devices, as protective layers in batteries, and as electrochemically active layers in solid-state batteries, fuel cells and gas separation membranes.

### CONTACT

Dr. Sven Uhlenbruck  
Tel: +49 2461 61-5984  
s.uhlenbruck@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# THERMAL COATING TECHNOLOGIES

Member of the Helmholtz Association



## THERMAL COATING TECHNOLOGIES

The team develops thermal coating technologies focusing on thermal spraying processes. Thermal spray techniques comprise coating processes in which surfacing materials are heated to the more or less plastic or molten state and then propelled onto a prepared surface. Powders, suspensions, or solutions are used as feedstock. The substrate remains unmelted. The energy carrier is a high-energy gas jet originating from compressed gas, from combustion of a gaseous or liquid fuel, from plasma generated by an electric arc discharge or a laser beam.

### THERMAL SPRAY PROCESSES

At IEK-1, various state-of-the-art industrial coating equipment is available, covering a wide range of materials and applications:

- Cold gas spraying (CGS), aerosol deposition (AD),
- High velocity oxy-fuel spraying (HVOF),
- High velocity air fuel spraying (HVOF),
- Atmospheric plasma spraying (APS),
- Low pressure plasma spraying (LPPS), LPPS-Thin Film (LPPS-TF), and plasma spray-physical vapor deposition (PS-PVD).

Thermal spraying can provide relatively thick coatings over a large area at high deposition rates. Coating materials include

- Alloys, e.g. MCrAlY, NiCr, stainless and ferritic steels, Inconel;
- Metals, e.g. tungsten, copper, titanium;
- Oxide ceramics, e.g.  $ZrO_2$ ,  $Al_2O_3$ ,  $TiO_2$ , spinels, pyrochlores (e.g.,  $Gd_2Zr_2O_7$ ), perovskites, aluminates;
- Non-oxide ceramics and composites, e.g.  $B_4C$ , WC/Co, MAX phases.

### PROCESS DIAGNOSTIC METHODS

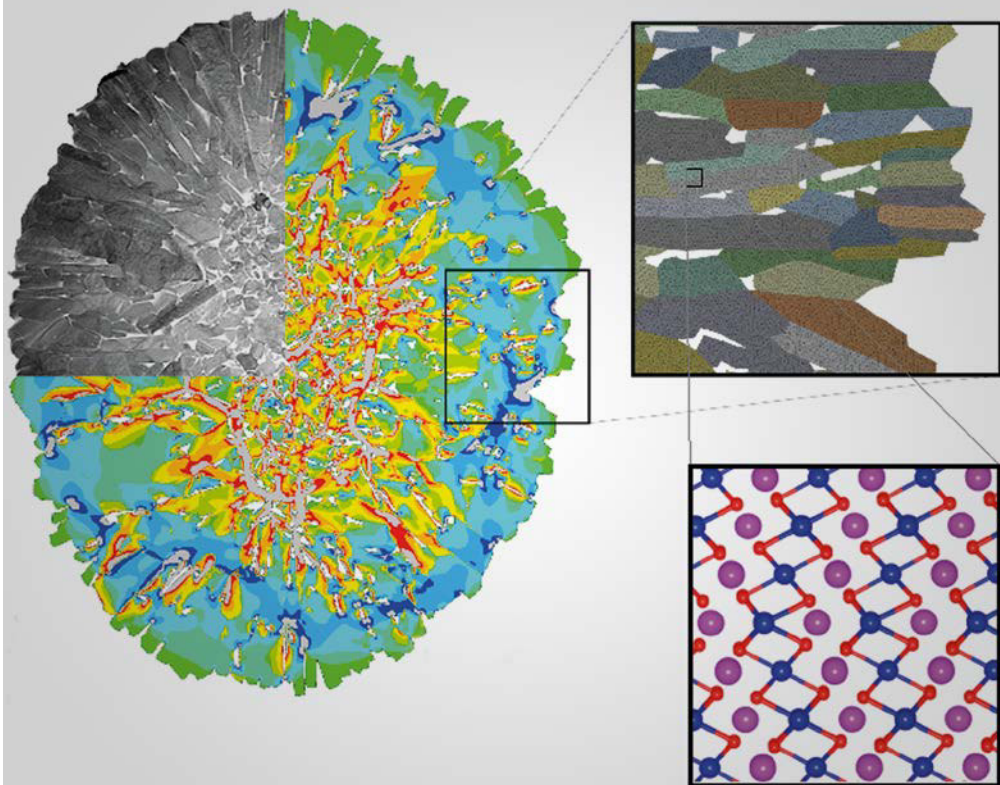
Plasma and particle in-flight characteristics are analyzed to gain understanding of the process and to manage quality:

- Plasma: enthalpy probe, optical emission spectroscopy;
- Particles: particle temperatures, velocities, and diameters, shadowgraphy of the particle flux;
- Stresses: in-situ measurement by curvature analysis.

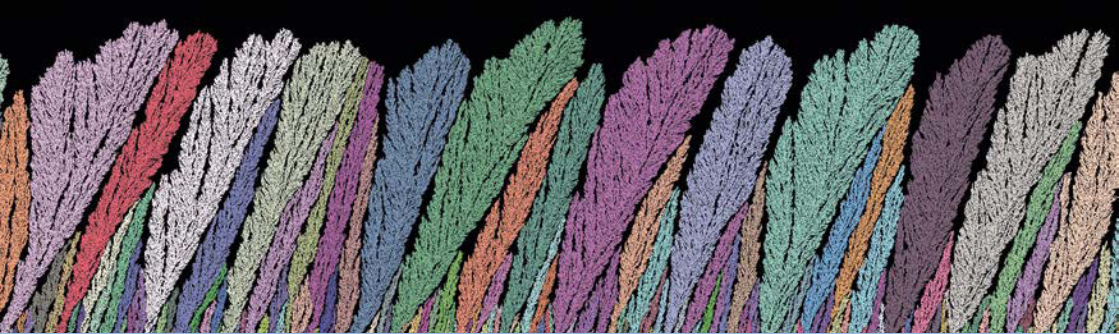
### CONTACT

PD Dr.-Ing. Georg Mauer  
Tel: +49 2461 61-5671  
g.mauer@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# MODELLING



## IMPROVED PROCESSINGS AND PROPERTIES OF MATERIALS BY MODELLING

The modelling team focuses on simulation of processing and properties of materials, in particular those which are interesting for energy conversion and storage systems. To achieve this aim, we develop and apply *ab initio* thermodynamics, kinetics, and dynamics as well as continuum approaches.

### PROCESSING

Modern processing routes require a good theoretical understanding of the underlying physical processes. With the help of theoretical descriptions and simulations, insights into the processes can be obtained that are crucial for the development towards manufacturing routes for well-designed materials with microstructures and properties required for the specific applications. This includes the simulation of flow fields of plasma jets with Computational Fluid Dynamics (CFD), the coupling of electrical, thermal, and mechanical fields during field assisted sintering with Finite Element Analysis (FEA), and the simulation of microstructure evolutions with Monte Carlo methods.

### PROPERTIES

The overall performance of a component is governed by its bulk, surfaces, grain boundaries, particles, and microstructure properties. For example, microstructural cracking of Li-ion battery cathodes is driven by non-monotonic lattice parameters changes of their crystal and instability of grain boundaries during charge/discharge. By combining first principles calculations and continuum mechanics simulations we can model and study the mechanism of crack formation in microstructures of cathode materials. Moreover, design parameters and microstructural or material properties are systematically varied and their impact on the operating performance are studied. This helps us to optimize the components which can then be produced experimentally.

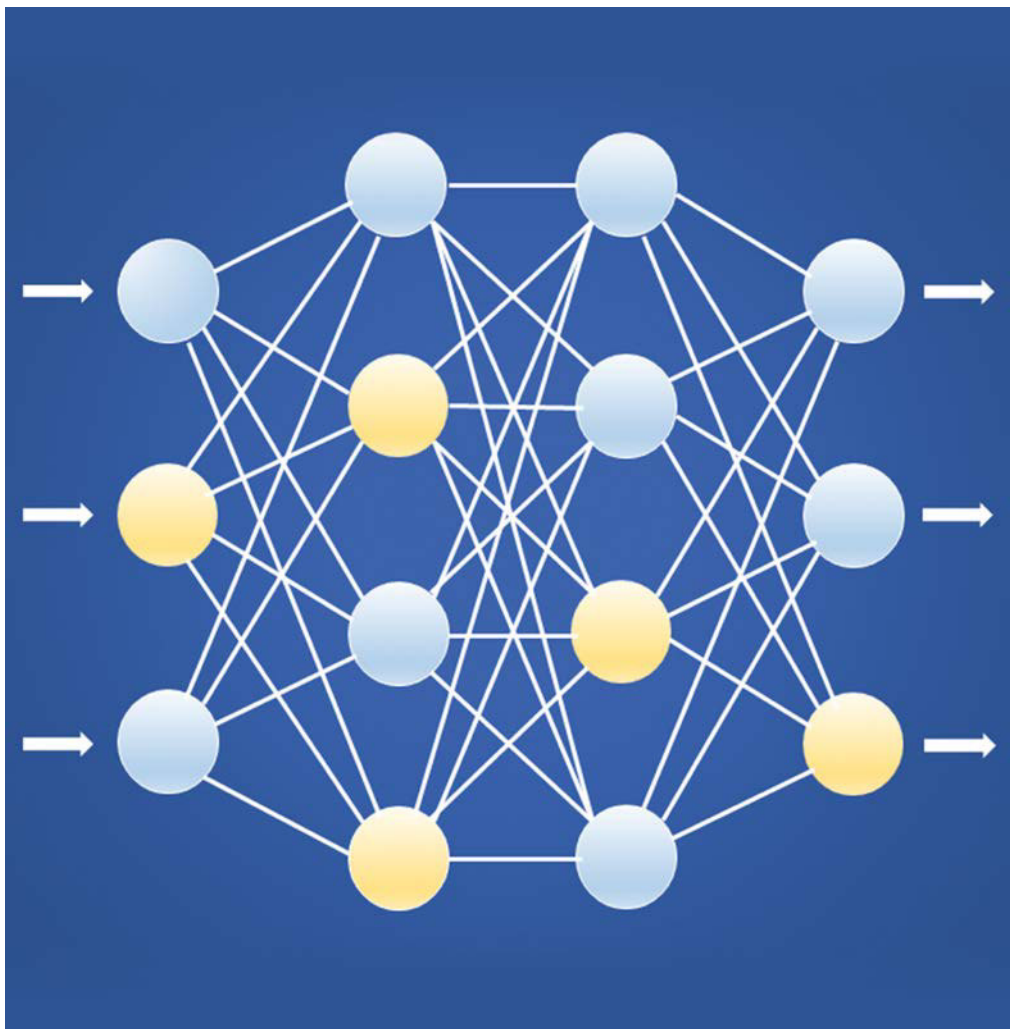
### INFRASTRUCTURE

Besides using external supercomputers, we run our own computing cluster (320 cores and 3.2 TB RAM) and different workstations. The most important thermo-mechanical material properties and sintering parameters can be measured with our own equipment.

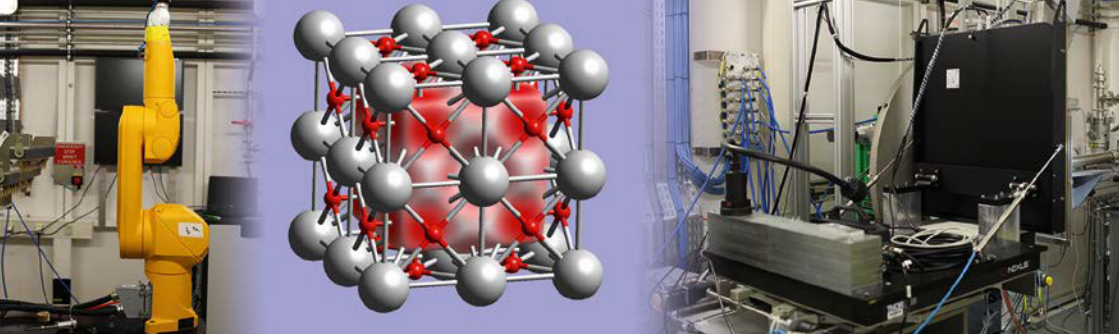
### CONTACT

Dr. Payam Kaghazchi  
Tel: +49 2461 61-4325  
[p.kaghazchi@fz-juelich.de](mailto:p.kaghazchi@fz-juelich.de)

EK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



## DATA-BASED MATERIALS DESIGN



## DATA-BASED MATERIAL DESIGN

The focus of the team entitled “Data-based material design” is on structural analyses with large-scale facilities, the development of structural models using simulation and modelling methods, and the analysis of chemical bonds in oxidic structures and their influence on the chemical and physical properties of ceramic materials. By applying machine learning and deep learning methods, new procedures for the digitalization of materials research are developed and the design of digital twins for fuel cells, gas separation membranes, solid state batteries and thermal protection layers is supported.

### STRUCTURAL SCIENCE AT LARGE-SCALE FACILITIES

Synchrotron radiation and neutron scattering methods are used for experiments on ceramics, in order to investigate their crystal and amorphous structures, including tomographic analyses, for the development of complete 3D models using large-scale equipment, e.g. at the ESRF (Grenoble) and DESY (Hamburg).

### RESEARCH DATA MANAGEMENT

New methods of research data management are introduced in order to enable the use of all available data for the development of digital twins. In this context, the team is working as a part of the National Research Data Infrastructure (NFDI), for IEK-1 and Forschungszentrum Jülich. NFDI supports researchers in the complete acquisition, analysis, processing, storage and publication of research data.

### APPLICATION OF ARTIFICIAL INTELLIGENCE IN MATERIALS SCIENCE

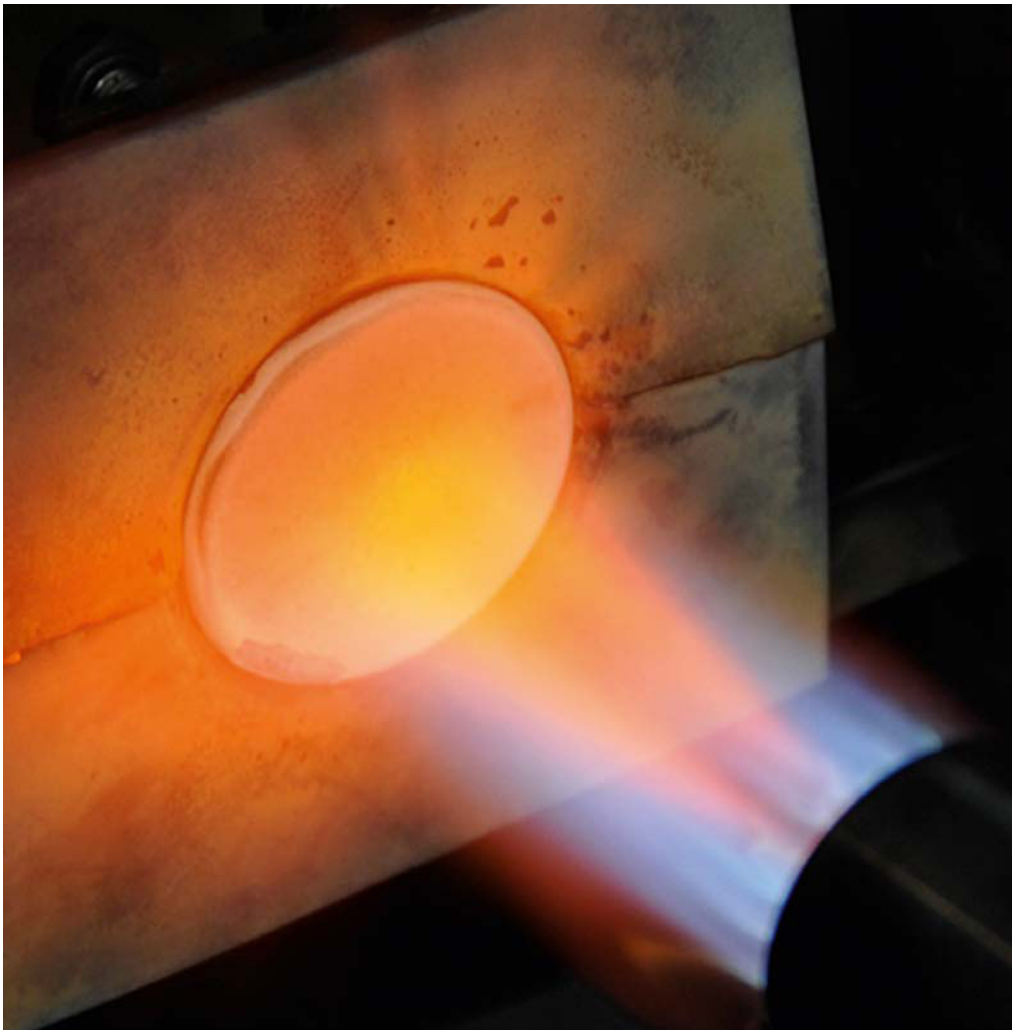
New Python machine learning and deep learning code is being developed to enable the virtualization of structure and material analytics and the prediction of material properties, which will eventually lead to the development of digital twins in order to shorten or save development time and costs. This work is carried out in cooperation with industrial partners and with specialist colleagues from other research centres.

### CONTACT

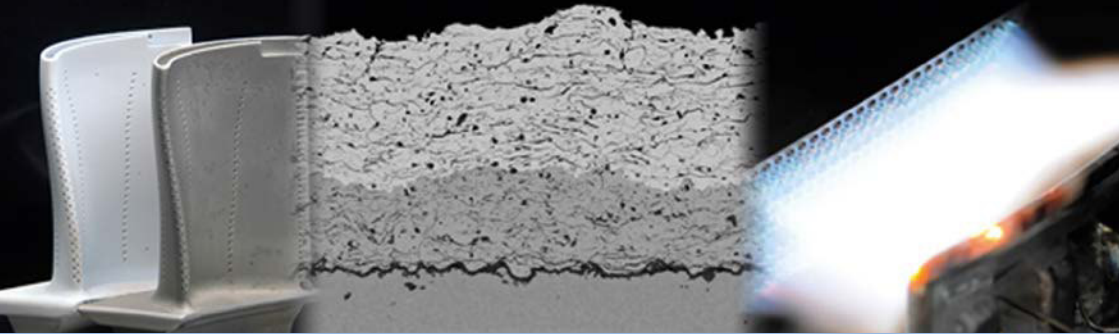
PD Dr. Hartmut Schlenz  
Tel: +49 2461 61-96956  
[h.schlenz@fz-juelich.de](mailto:h.schlenz@fz-juelich.de)

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany





# HIGH TEMPERATURE PROTECTIVE COATINGS



## COATINGS FOR EXTREME ENVIRONMENTS

The team focuses on developing materials solutions for protective coatings such as thermal barrier coatings (TBC) and environmental barrier coatings (EBC) for highly thermomechanically loaded components, primarily in stationary and aircraft gas turbines. In order to ensure fast development cycles, special emphasis is given to the assessment of their functionality and lifetime at high temperatures under realistic test conditions (e. g. in burner rig testing).

### ADVANCED MULTILAYERED EBCS AND TBCS

Starting from the specification and synthesis of new, mainly ceramic materials, components with TBCs and EBCs based on advanced multilayered and/or graded architectures are manufactured. The application of new processing technologies allows for the development of EBC/TBC systems with well-controlled properties in terms of microstructure and local composition. Pyrochlores such as  $Gd_2Zr_2O_7$ , complex perovskites or (hexa)aluminates are of particular interest for TBC applications. Due to

their relatively low fracture toughness, double-layer systems developed at IEK-1 are usually required. Research on EBCs currently focuses on rare-earth silicates and other oxides. For the improvement of adhesion of thick coatings on inhomogeneous substrates such as ceramic matrix composites or abradables, advanced laser surface texturing is employed.

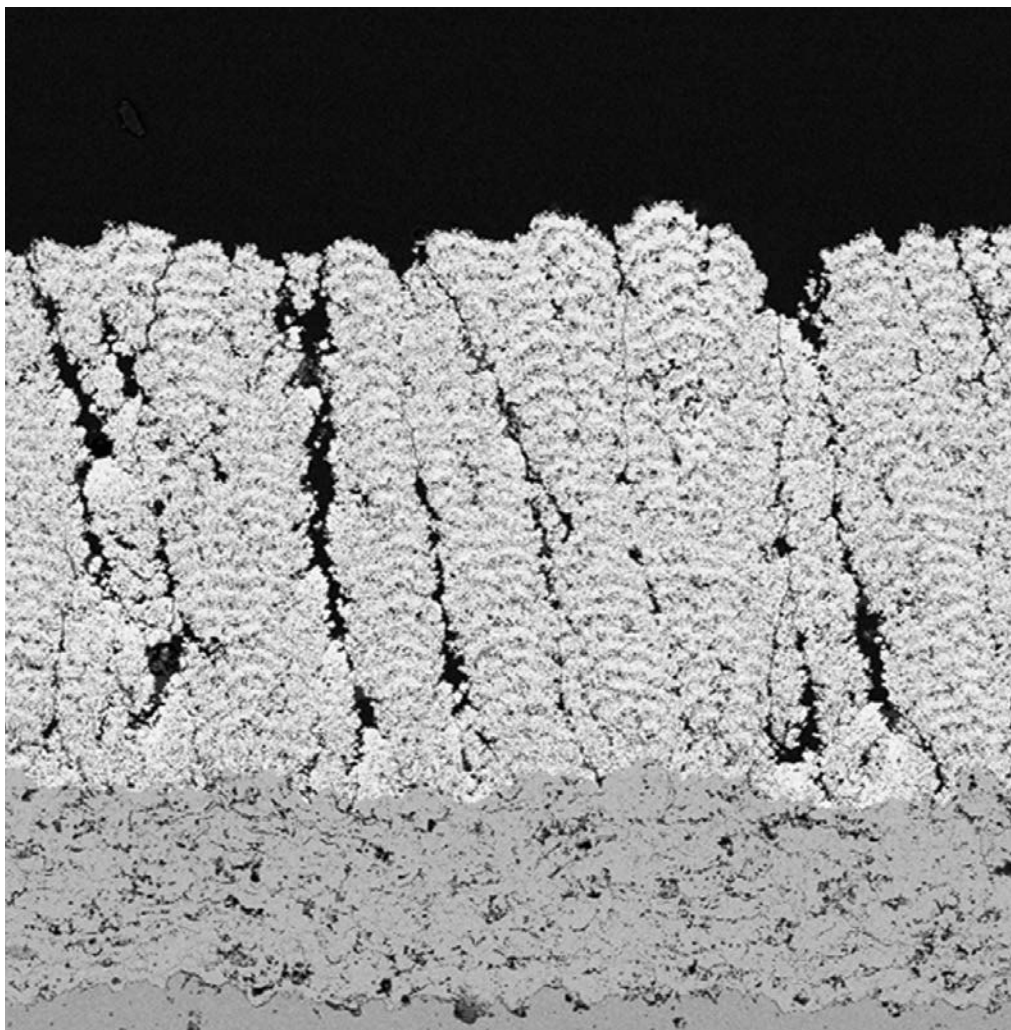
### TBCS RESISTANT TO MOLTEN DEPOSITS

An increasingly important aspect at even higher temperatures is the resistance of porous layers against infiltration by calcium-magnesium-aluminium silicates (often called “CMAS”). These silicates are present in air as solids and are also produced by abrasion in the rephrase. They are deposited on the turbine components and can penetrate the barrier coatings in their molten form. Once they solidify, they cause considerable damage by decreasing the strain tolerance. In addition to the Gd-containing pyrochlores, aluminates also show a better stability than YSZ.

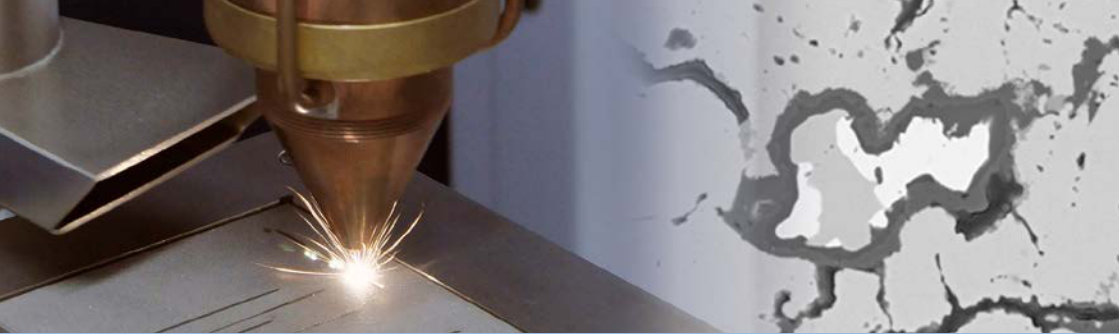
### CONTACT

Dr. Daniel E. Mack  
Tel: +49 2461 61-2971  
d.e.mack@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



## SMART COATINGS



## ADVANCED FUNCTIONAL COATINGS

The team develops layer systems with additional functional properties such as sensing properties, self-healing capabilities or enhanced strain tolerance. In addition, the team combines the achievements of the high temperature protective coating and the thermal coating technology teams. A further activity is the development of functional layers for gas separation applications or for solid oxide fuel cells. Furthermore, innovative coating processes especially suitable for functional coatings, such as the aerosol deposition process, are developed.

### ADDITIONAL FUNCTIONALITIES IN HIGH TEMPERATURE COATINGS

Sensing properties are added into YSZ based thermal barrier coatings (TBCs) using an adapted laser cladding process for the deposition of thermocouple clads without degrading the TBC structure. Embedding is then achieved by a subsequent deposition on YSZ by an atmospheric plasma spraying process (APS). Other sensors, such as strain sensors, can also

be produced via this approach. Self-healing TBCs can be produced by adding specific  $\text{MoSi}_2$  powders into the YSZ TBC layer. An adaption of the APS process is necessary to avoid the decomposition of the  $\text{MoSi}_2$  powder. This approach can also be used for other protective coating systems.

### STRAIN-TOLERANT COATING SYSTEMS

The team is using suspension plasma spraying (SPS) and plasma spray physical vapor deposition (PS-PVD) techniques to develop columnar structured coatings with extreme strain tolerance.

### DENSE FUNCTIONAL COATINGS

The team uses advanced thermal spray techniques to produce different functional coatings with high gas-tightness e.g. for applications as oxygen or hydrogen separation membranes, as electrolytes in solid oxide fuel cells (SOFCs) or as chrome evaporation barriers in SOFCs. In addition the developments are used to produce environmental barrier coatings (EBCs)

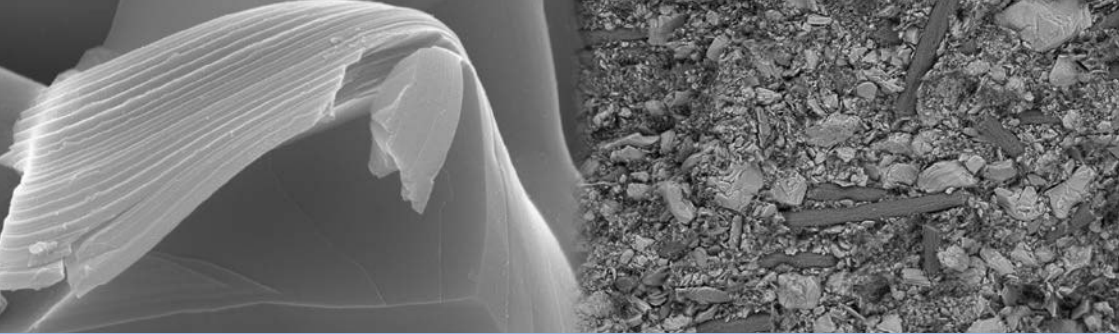
### CONTACT

Prof. Dr. Robert Vaßen  
Tel: +49 2461 61-2455  
r.vassen@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



## CERAMIC COMPOSITES



## CERAMIC MATRIX COMPOSITES

The team develops novel Ceramic Matrix Composites (CMCs) for systems that operate at high temperature and harsh environmental conditions, such as gas turbine components or Concentrated Solar Power (CSP) units. The composites are based on MAX phases as matrices, a novel family of materials that bridges the gap between ceramics and metals. Among all the MAX phases, we mainly focus on  $\text{Cr}_2\text{AlC}$ ,  $\text{Ti}_3\text{SiC}_2$ ,  $\text{Ti}_2\text{AlC}$  and  $\text{Ti}_2\text{AlN}$  due to their excellent oxidation/corrosion resistance and good mechanical properties. Regarding the reinforcing phase,  $\text{SiC}$  and  $\text{Al}_2\text{O}_3$  fibers are mainly used.

### PROCESSING OF COMPOSITES

The scope of the team includes the synthesis of MAX phase powders, processing of different structures and their densification. Pure MAX phase powders are obtained by two different synthesis routes: a novel process referenced as Molten Salt Shielded Synthesis (MS3) and by solid-liquid state reaction. Scaling up these processes leads to kilograms of high-quality powder per batch, which is required to develop complex and large components as well as

to facilitate the transferring of these new materials to industry. Based on our expertise in ceramic processing, we are able to develop different structures, from dense components and coatings by Thermal Spray Technologies as Cold Spray (CS) and High Velocity-Atmospheric Plasma Spray (HV-APS) to porous foams and near net shapes by Ceramic Injection Molding (CIM) and Additive Manufacturing (AM).

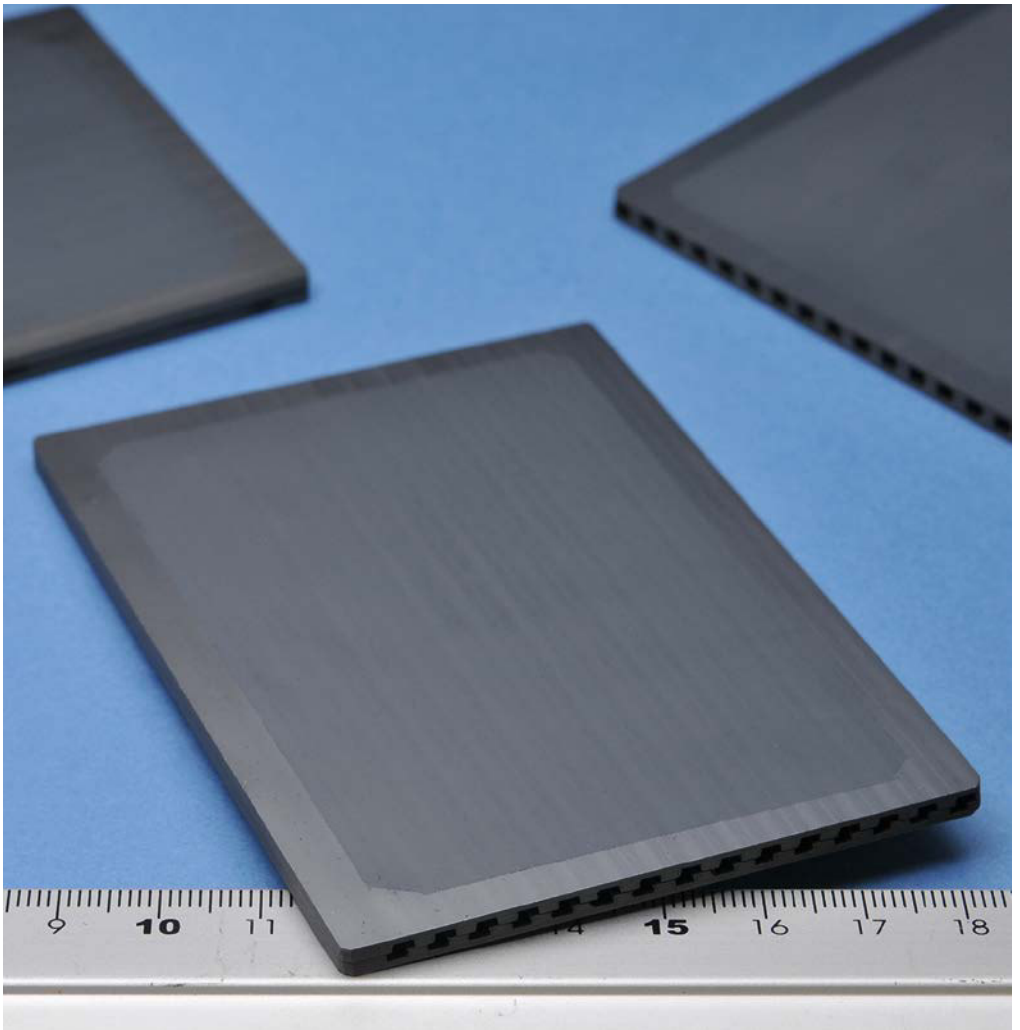
### HIGH TEMPERATURE RESPONSE

Developed CMCs are tested under realistic and aggressive environmental conditions, similar to those that the final components will withstand. Due to the novelty of MAX phases, their oxidation and corrosion resistance under different environmental conditions has not been explored sufficiently. Long term experiments at high temperature (1000 °C – 1300 °C) using burner rigs, thermal shock tests, characterization of the interaction of the CMCs with Thermal Barrier Coatings (TBCs), and mechanical characterization – flexural strength, tension and compression creep – are thus among the interests of the team.

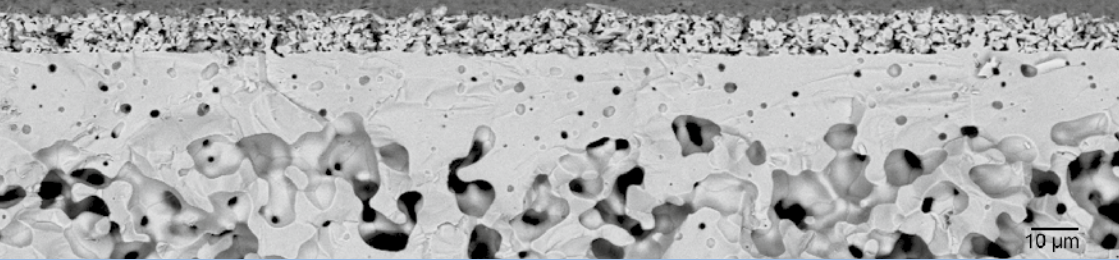
### CONTACT

Jun.-Prof. Dr. Jesus Gonzalez  
Tel: +49 2461 61-96761  
[j.gonzalez@fz-juelich.de](mailto:j.gonzalez@fz-juelich.de)

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



## OXYGEN-PERMEABLE MEMBRANES



## OXYGEN PERMEABLE MEMBRANES

Oxygen transport membranes (OTM) provide an efficient way to separate oxygen from air at elevated temperatures, i.e. 500 – 900 °C. It is possible to either generate pure oxygen for any purpose, e.g. combustion processes, metallurgy, or medical applications, or to utilize the separated oxygen directly in chemical reactions such as partial oxidation of hydrocarbons to produce commodity chemicals.

### OTM MATERIALS

OTM materials are ceramics showing mixed ionic-electronic conductivity (MIEC). This process does not consume any energy, making it very efficient. However, temperatures above 500 °C are necessary to realize fast ion diffusion. The selection of a suitable material depends highly on the operation conditions (particularly temperature, pressure and atmosphere), which are defined by the target application. IEK-1 thus established a materials tool box.

Perovskite-type oxides often show MIEC behaviour (e.g.  $\text{La}_{1-x}\text{Sr}_x\text{Co}_{1-y}\text{Fe}_y\text{O}_{3-\delta}$  or  $\text{SrTi}_{1-x}\text{Fe}_x\text{O}_{3-\delta}$ ).

But the transport process relies on crystal defects creating a trade-off between permeability and stability. Therefore, composite materials composed of a pure ionic (e.g.  $\text{Ce}_{0.8}\text{Gd}_{0.2}\text{O}_{2-\delta}$ ) and a pure electronic conductor (e.g.  $\text{FeCo}_2\text{O}_4$ ) are also under investigation, enabling the use of inherently stable material combinations.

### OTM COMPONENTS

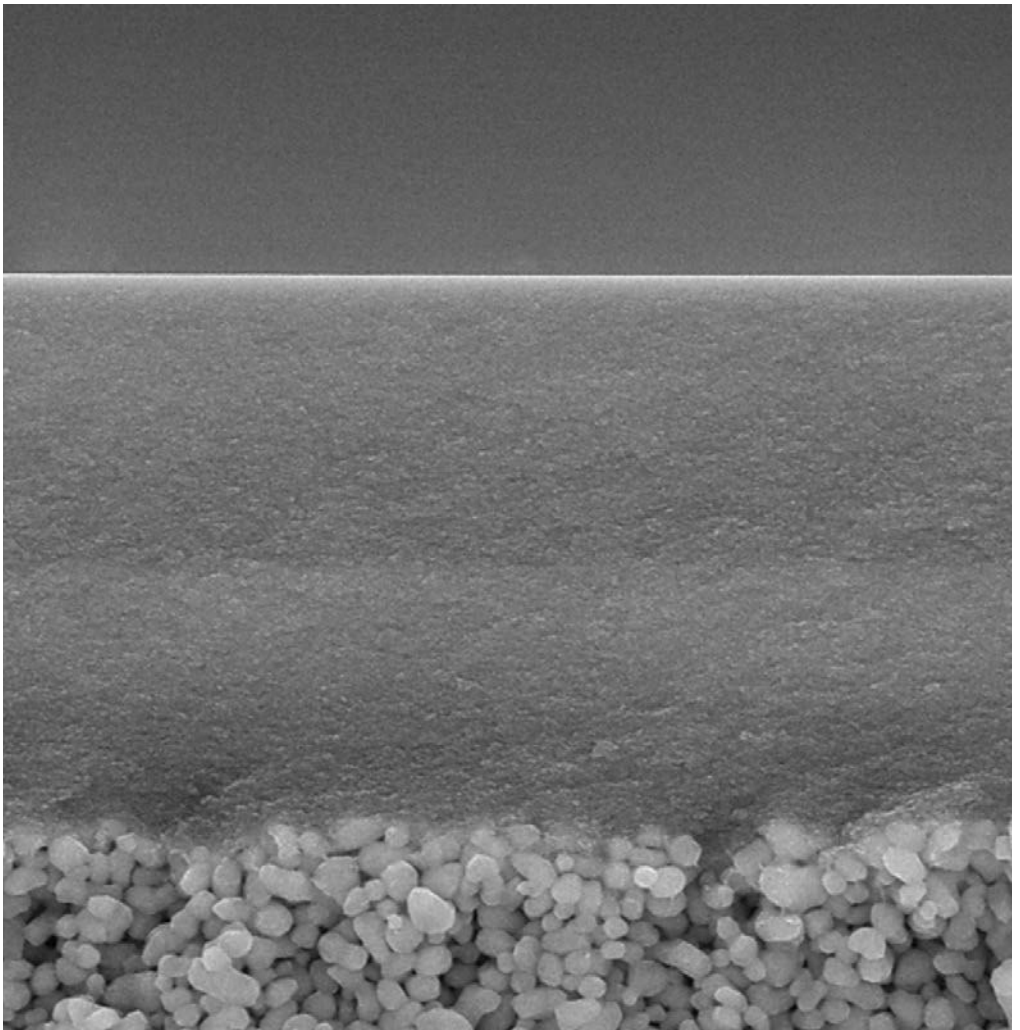
Optimized membranes should be as thin as possible, requiring a mechanically stable support with sufficient porosity in order to enable oxygen feed to the thin membrane layer. Ideally, fine porous surface activation layers at both sides of the membrane facilitate oxygen surface exchange. For this purpose, IEK-1 relies on ceramic manufacturing technology suitable for mass production, particularly tape casting and screen printing, complemented by modelling efforts. In addition, novel processing technologies such as freeze casting and 3D-printing are being explored. A novel thermal spray technology has been developed for the coating of OTM on robust metallic supports, which is exceedingly challenging.

### CONTACT

Dr. Stefan Baumann  
Tel: +49 2461 61-8961  
s.baumann@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany





# **HYDROGEN-PERMEABLE MEMBRANES**



## HYDROGEN-PERMEABLE MEMBRANES

The team Hydrogen-Permeable Membranes develops dense and microporous ceramic membranes able to transport hydrogen, either in protonic ( $H^+$ ) or molecular form ( $H_2$ ) by means of selected materials and advanced fabrication techniques. Different transport mechanisms, the chemical nature of membrane materials, or process conditions allow for various application areas ranging from separation tasks (extraction of highly pure  $H_2$  from gas mixtures) to intensifying complex chemical reactions in catalytic membrane reactors using e.g.  $H_2$  and  $CO_2$  or  $N_2$  to form bio-fuels, higher hydrocarbons, or ammonia, respectively. In addition the separation of different other gas species from mixtures and the dehydrogenation of alcohols via pervaporation is a focus of the group. This is based on micro- and mesoporous membranes based on silica-carbon bonds, graphen and zirconia.

### FABRICATION TECHNIQUES AND MATERIALS

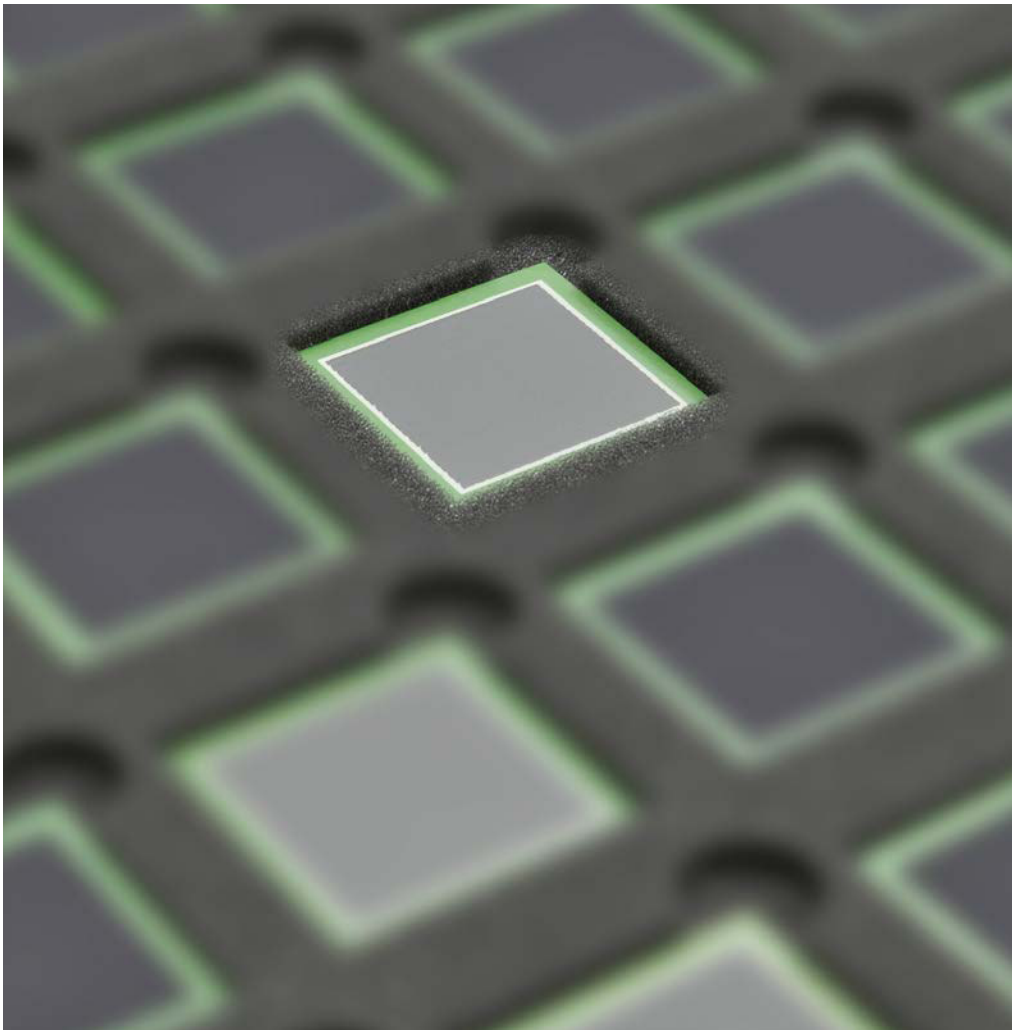
Membranes of different thicknesses (nm- $\mu$ m range), microstructure and final geometries

are fabricated on either ceramic or metallic substrates by means of advanced, reproducible and scalable fabrication techniques, e.g. tape casting, screen printing, spin and dip coating in a clean room, PS-PVD etc. In addition, their properties are thoroughly studied by various characterization methods. The selection of materials covers several structural classes, ranging from well proven conventional choices such as graphene or zirconates and cerates with perovskite structure to novel, patented compositions such as rare-earth tungstates with defective fluorite structure. Along with the development of defect-free and highly performing membranes for the targeted energy and environmental applications, the team carries out detailed fundamental research on the interplay between composition, microstructure, performance and stability, partnering with a strong network of universities and research institutions under numerous national and international projects or other collaboration initiatives.

### CONTACT

Prof. Dr. Wilhelm A. Meulenberg  
Tel: +49 2461 61-6323  
[w.a.meulenberg@fz-juelich.de](mailto:w.a.meulenberg@fz-juelich.de)

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# SOLID OXIDE CELLS



## SOLID OXIDE FUEL AND ELECTROLYSIS CELLS

The department of Solid Oxide Fuel and Electrolysis Cells (SOFC and SOEC) concentrates on material development and manufacturing methods for solid oxide fuel and electrolysis cells, mainly based on ceramic powder processing. The main focus is the development of new materials and the optimization of the microstructure of functional components.

### **BEING PART OF THE FUTURE ENERGY SYSTEM**

At IEK-1, SOC research focuses on cells, contact layers and interconnect protective layers. Research and development starts with the synthesis of suitable materials or the purchase of commercially available powders and their conditioning: ranging from raw materials and intermediate products (slips, pastes, suspensions), layers, components, and parts to scaling up in terms of component size, homogeneity, and reproducibility as appropriate for application in a pilot plant. For the manufacturing processes, mostly powder-based methods from metal and

ceramic powder processing are applied, such as pressing, tape casting, screen printing, or wet spraying. If certain properties are required for functional layers, thin-film processes (PVD, sputtering), precursor-based techniques such as sol-gel processes (spin or dip coating, inkjet printing) and thermal spray technologies may also be applied. Studies on the degradation of SOCs and intensive post-test analyses of fuel cell stacks round out the research portfolio.

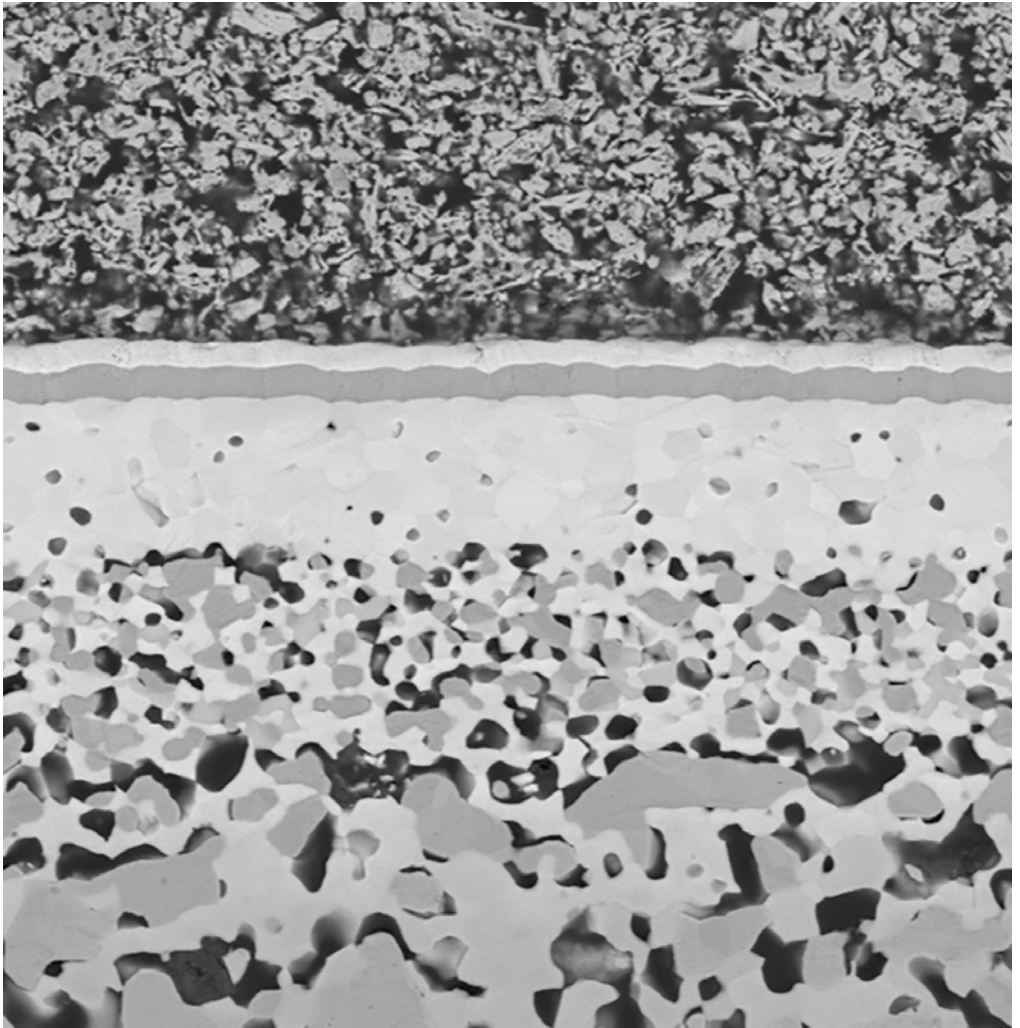
### **ENABLING EASY ACCESS TO ENERGY FOR EVERYONE**

In addition to our long-standing expertise in SOFC research, we work on high-temperature electrolyzers to produce hydrogen in steam electrolysis or syngas in co-electrolysis and on high-temperature metal-air batteries, storing energy by oxidation/reduction of metal (e.g. iron) incorporated into the fuel compartment. The focus is on the development of adapted electrodes for cells, characterization and post-test analysis of solid oxide electrolysis stacks.

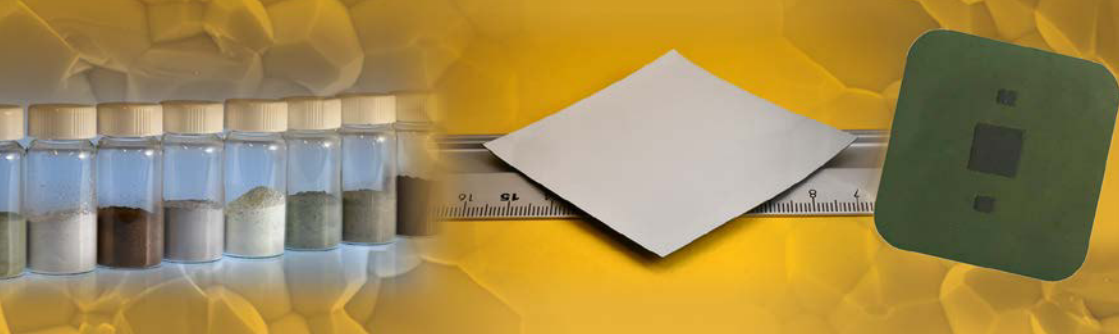
### **CONTACT**

Hon.-Prof. Dr. Norbert H. Menzler  
Tel: +49 2461 61-3059  
[n.h.menzler@fz-juelich.de](mailto:n.h.menzler@fz-juelich.de)

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany



# LOW TEMPERATURE SOLID OXIDE CELLS



## LOW TEMPERATURE SOLID OXIDE CELLS

Low Temperature Solid Oxide Cells (LT-SOC) are electrochemical energy conversion devices operating in the temperature range of 400°C to 600°C, which convert chemical fuels to electricity (fuel cell mode) or generate hydrogen from water under surplus energy consumption (electrolysis mode). Such electrochemical devices are excellent systems for the generation of electricity due to their fuel flexibility ( $H_2$ ,  $C_x H_y$ ), as well as a key element of electrical energy storage systems based on power-to-gas technology, and the  $H_2$  based economy of the future.

### OUR COMPETENCE

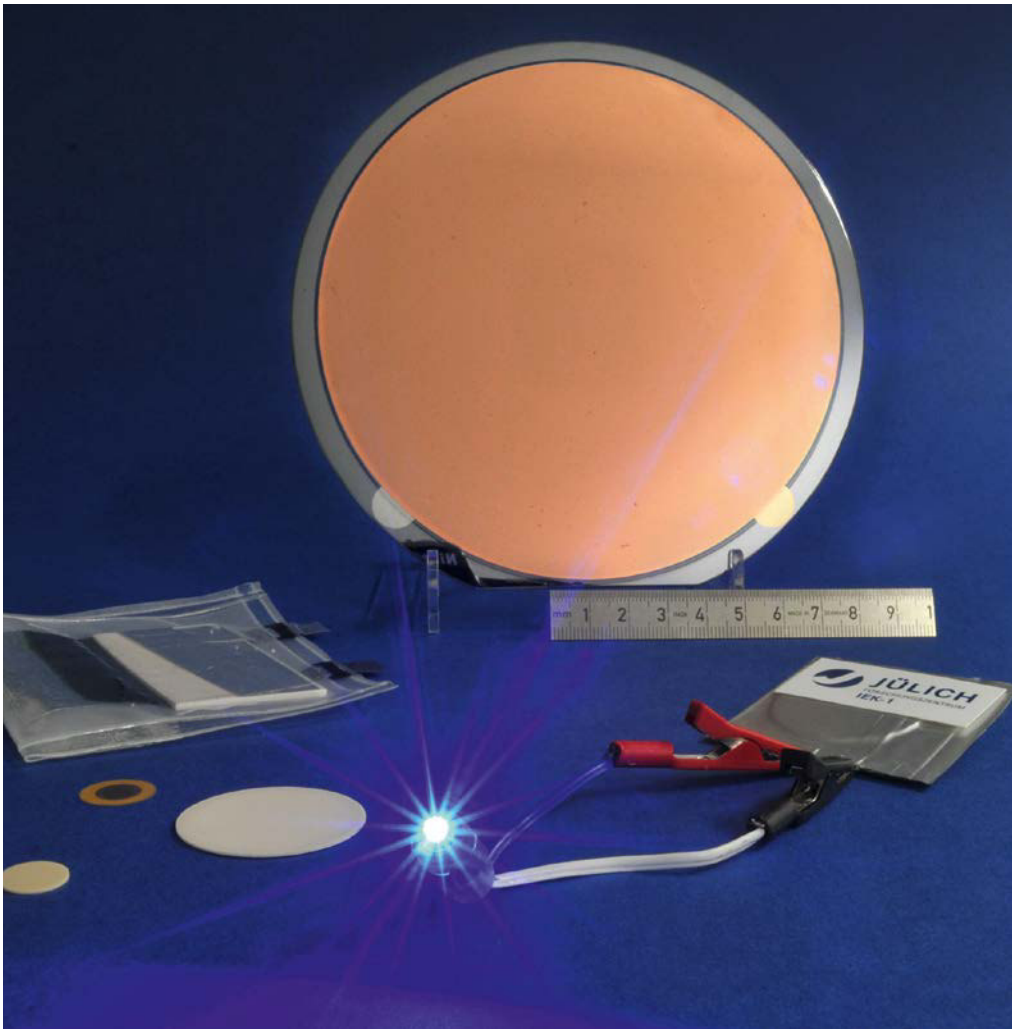
Our portfolio aims at systematic research and development of LT-SOC based on both proton conductors and oxygen ion conductors in order to increase the readiness of this technology for the market. Proton- and oxygen ion conducting

ceramics are both viable choices for achieving the LT-SOC target performance at decreased operation temperature, while exhibiting reasonable stability and durability under steam conditions. For that, we focus on improving the overall performance, long-term stability, durability and scalability of these electrochemical devices. As the LT-SOC is a multi-layered ceramic system, we develop ceramic materials with tailored properties required for their specific function in the cell (solid electrolyte, cathode, anode, interconnect contact and protective coating), and we combine these materials to shape cell components with high compatibility and designed interfaces. Finally, we fabricate LT-SOCs with tailored microstructure and scalable geometries by means of leading processing technologies and we investigate their integration and operation in the Jülich stack design.

### CONTACT

Proton conducting SOC  
Dr. Mariya E. Ivanova  
Tel: +49 2461 61-5149  
[m.ivanova@fz-juelich.de](mailto:m.ivanova@fz-juelich.de)

Oxygen ion conducting SOC  
Dr. Christian Lenser  
Tel: +49 2461 61-5357  
[c.lenser@fz-juelich.de](mailto:c.lenser@fz-juelich.de)



# SOLID-STATE BATTERIES



## SOLID-STATE BATTERIES – MANUFACTURING AND ANALYSIS

New fields of application in electro-mobility and stationary energy storage drive the development of battery technology while in established fields of application, requirements with respect to safety, energy and power density also increase steadily. Thus, the application-targeted investigation of new, disruptive concepts combined with strategies to ensure transferability of the results into industry are the focal points of the solid-state batteries team at IEK-1.

### SOLID ELECTROLYTES AND SEPARATORS

One option to enhance the safety as well as the energy and power density is the shift from liquid or polymer electrolytes to ceramic ones. Scalable fabrication of ceramic materials with high electrochemical stability, ionic conduction at room temperature and compatibility with the other cell components is essential here.

Separators and multi-layered structures made from these materials can also be applied in other next-generation batteries, such as metal-air, metal-sulphur, metal-ion, etc.

### HIGH CAPACITY MIXED CATHODES

To obtain high energy densities on the cathode side, the processing of ceramic electrolytes with specific (high voltage) active materials needs to be optimized. Chemical stability during processing and low interface resistances are needed for superior cell performance.

### METAL ANODES

Metal anodes are the goal for almost all next-generation battery systems, but can only be used at relevant current densities if dendrites are prevented. Intrinsic dendrite prevention by materials design and protective concepts (e.g. interlayers) are our main strategies to enable metal anodes.

### ANALYSIS

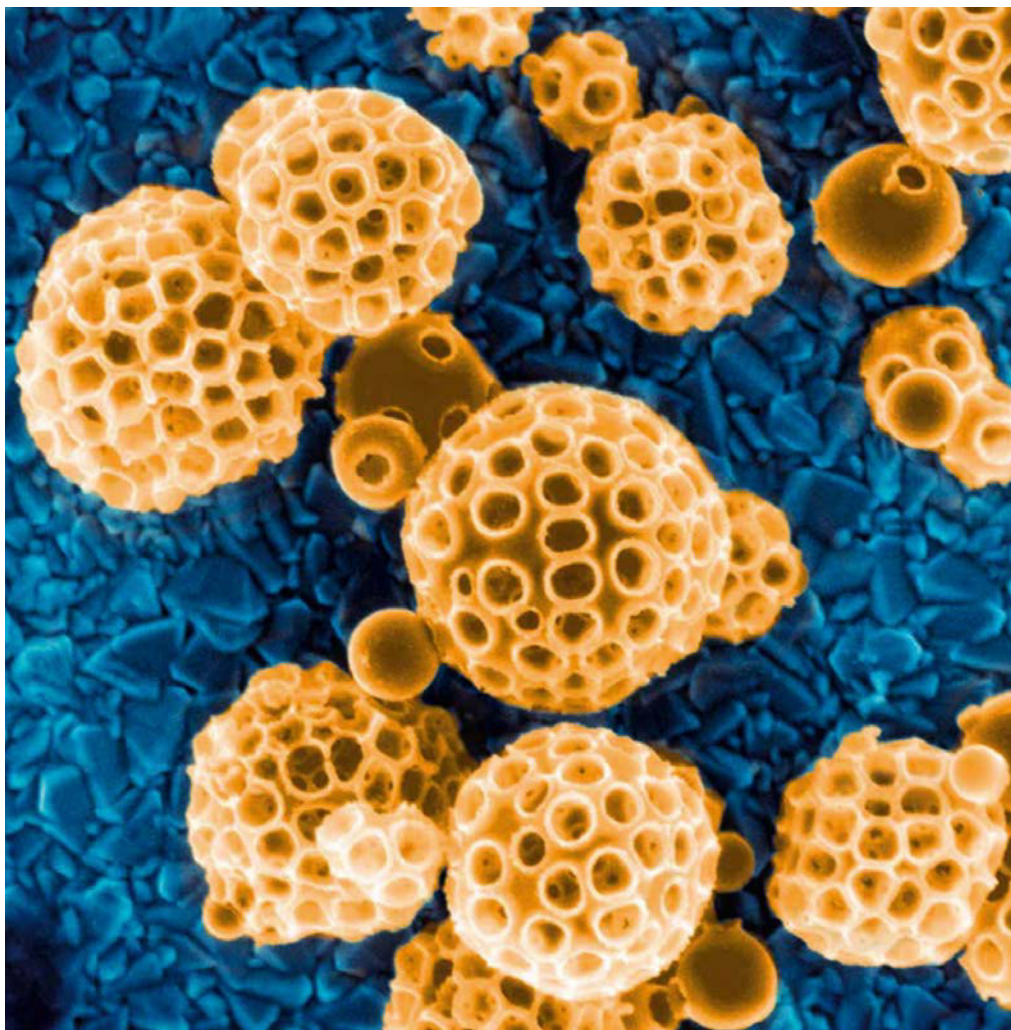
For targeted cell development, advanced 2-D and 3-D analysis methods based on ion beams (SIMS, RBS, NRA) are developed for in-situ and operando measurements of components and cells. Quantification of Li and other trace elements is key to enable fast design-performance optimization loops.

### CONTACT

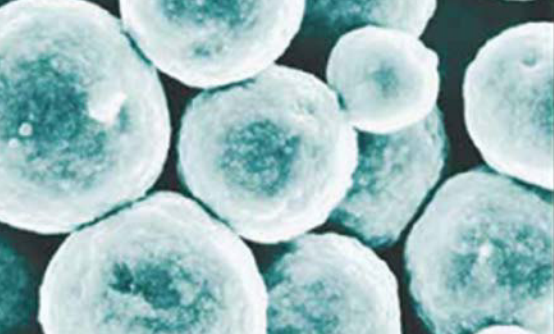
Dr. Martin Finsterbusch  
Tel: +49 2461 61-2877  
m.fensterbusch@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany





# ELECTROACTIVE NANOMATERIALS



## ELECTROACTIVE NANOMATERIALS

Fast charging batteries, more efficient electrocatalysts: The team “Electroactive Nanomaterials” aims at the development of novel optimized morphologies of materials for energy conversion and storage applications and understanding the processes influencing charge transport properties on the nanoscale.

### GENERAL SCOPE

We explore chemical strategies for the fabrication of ultrasmall metal oxides nanoparticles using aqueous and non-aqueous synthesis routes, as well as defined 3D-scaffolds with a high interface area and a continuous charge transport pathways. Our current projects include iridium-based electrocatalysts for polymer electrolyte membrane (PEM) water electrolysis with a minimized Ir content, and electrode morphologies for Li-ion batteries.

### BATTERY ELECTRODES

An increasing need for high energy density and fast charging Li-ion batteries demands the development of novel electrode morphologies. Our

team works on  $\text{SnO}_2$ -based conversion/alloying-type anodes and high voltage olivine-structured cathodes  $\text{LiMPO}_4$  ( $M = \text{Fe}, \text{Mn}, \text{Co}, \text{Ni}$ ) that feature high energy densities but suffer from various drawbacks such as high volume changes or low electronic conductivity. To improve the electrode performance we use a combination of morphology optimization (such as nanoscaling and the formation of hybrids with carbonaceous conducting materials) and changing bulk properties via doping with different ions.

### ELECTROCATALYSIS

PEM electrolysis enables sustainable generation of hydrogen with high efficiency, but the large scale application is currently limited by the high cost of its components and in particular iridium used to catalyze the oxygen evolution reaction (OER) process. We develop scalable approaches to prepare dimensionally stable OER catalyst with a very low Ir volumetric loading density but high OER activity by developing complex porous conductive oxide supports ( $\text{TiO}_2$ - and  $\text{SnO}_2$ -based) and conformally coating them with small  $\text{IrO}_2$  nanoparticles.

### CONTACT

Prof. Dina Fattakhova-Rohlfing  
Tel: +49 2461 61-85051  
d.fattakhova@fz-juelich.de

IEK-1: Materials Synthesis and Processing  
Forschungszentrum Jülich GmbH  
52425 Jülich, Germany