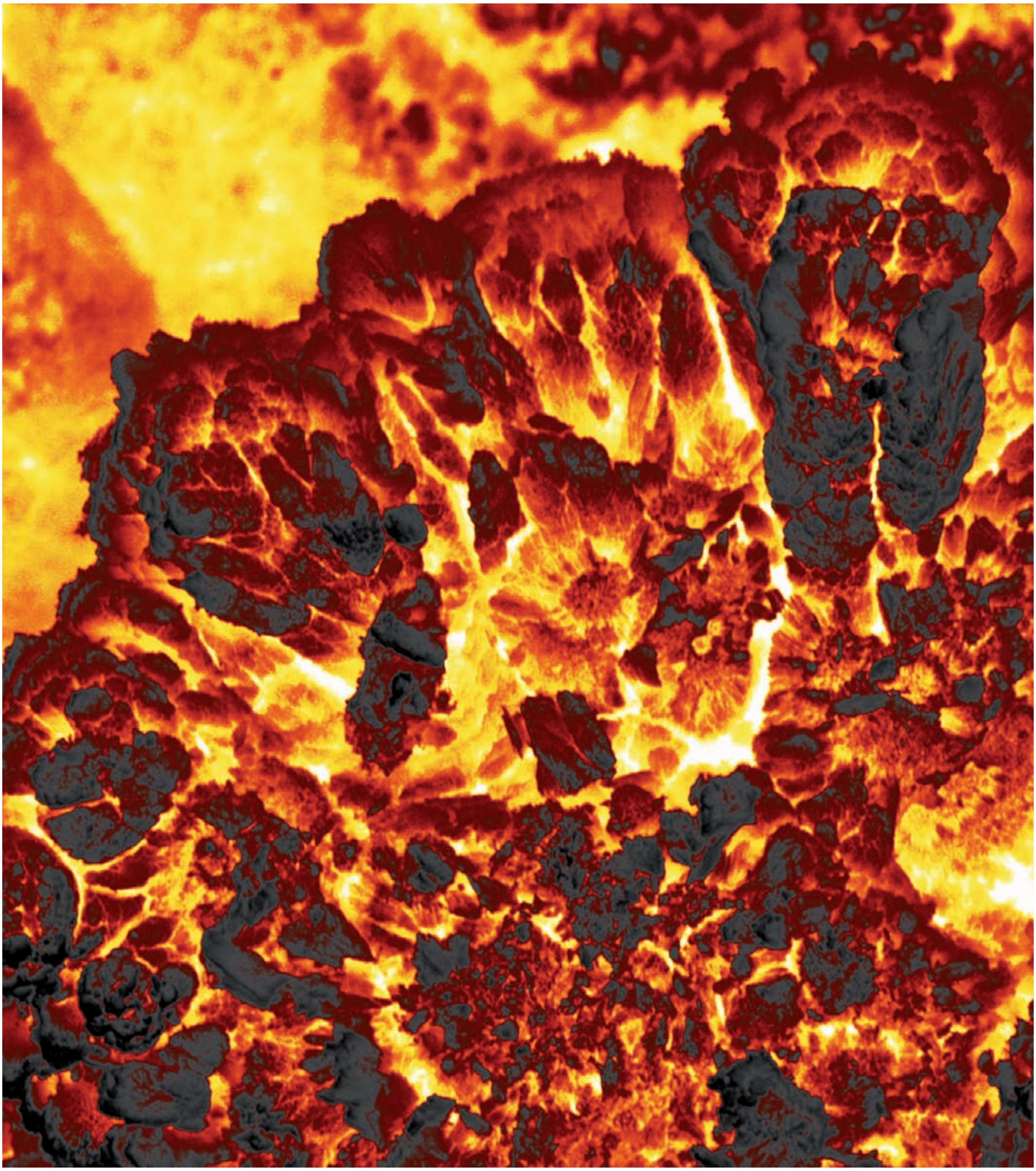
10 minus 9

HIGHLIGHTS OF NANOSCIENCES AT
THE UNIVERSITY OF DUISBURG-ESSEN

ISSUE 1/2019

CENIDE
CENTER FOR NANOINTEGRATION
DUISBURG-ESSEN



Cover: Lava stone (colored afterwards): Using a picosecond laser, the surface of a piece of stainless steel was structured and thus increased 50-100 times. In this case, the piece of stainless steel serves as an in situ XPS specimen holder. Due to the structuring, the laser beam for heating the sample can be well absorbed. Shot in SE mode. Magnification: 9,600x. The laser structuring was done by cooperation partners at the „Forschungszentrum für Energiespeichertechnologien“ at the TU Clausthal. (Photo: Simon Siebeneicher, AG Reichenberger/Barcikowski)

Left: Prof. Dr. Heiko Wende,
Scientific Director.
Right: Dr. Tobias Teckentrup,
Managing Director.

Dear members and friends of CENIDE,

More science, more facts, less annual report. In a nutshell, that's the most important things when changing from "CENIDE compact" to "10 minus 9". And the layout, of course: It is more modern, in a magazine-like style. We hope you like it. From now on, "10 minus 9" will be published every two years and will alternate with the research report on the UDE's key research profile areas.

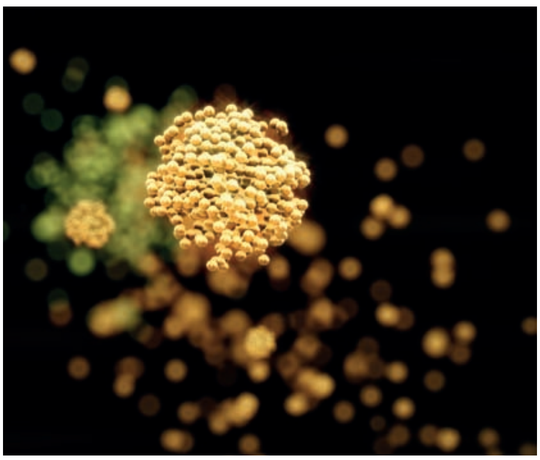
It was about time for a change of content and style in CENIDE's very own publication, because after almost 15 years, our network is anything but "nano": 74 working groups currently belong to CENIDE; trend still rising. And just as at a celebration with many guests, who are grouped in appropriate table groups for better communication, the division into six main research areas is therefore both sensible and necessary: (1) Catalysis, (2) Dynamic processes in solids, (3) Gas-phase synthesis of nanomaterials, (4) Magnetic materials, (5) Nanomaterials for health, and (6) Nanotechnology in energy applications. The scientific highlights and milestones achieved in these topics over the past two years make up the core of this journal. Together with numerous joint projects, proposals and cooperations they impressively demonstrate that the teamwork functions.

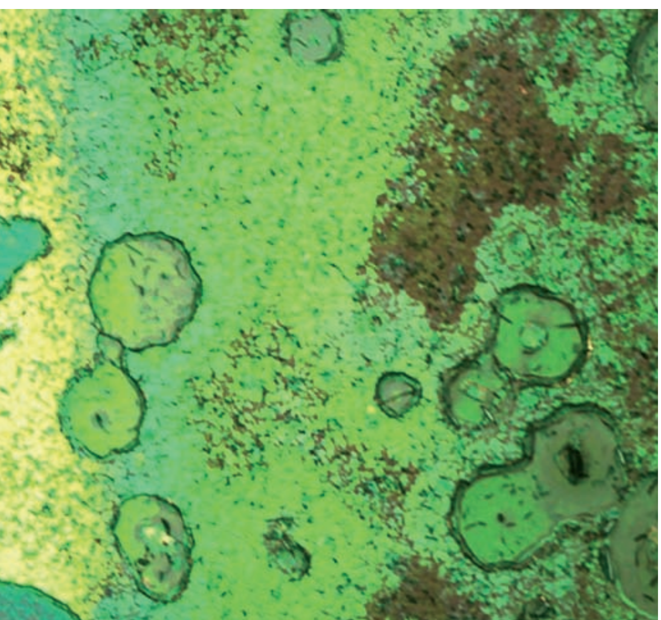
CENIDE is an interdisciplinary network based on the exchange with colleagues from related disciplines and the resultant impetus from a different perspective. Regular events such as the CENIDE conference, numerous symposia and workshops make sure of this.

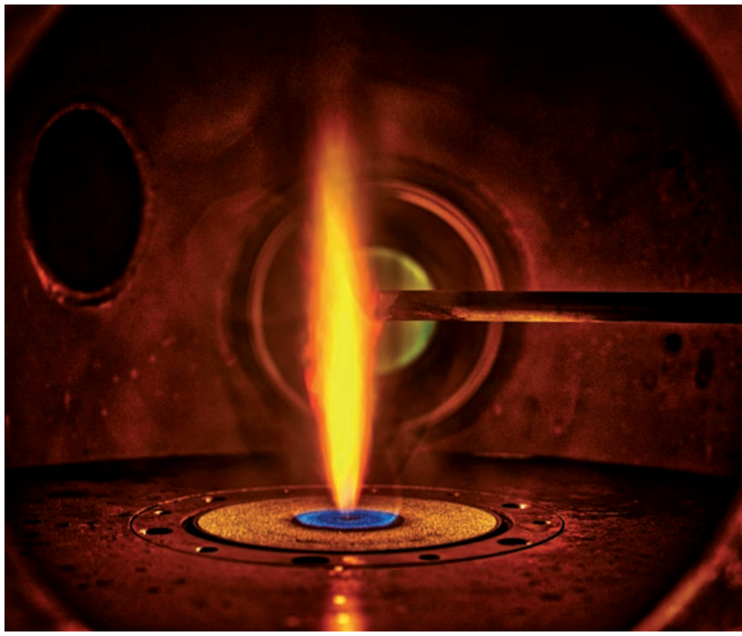
Therefore, we would particularly like to thank you for your active and constructive contribution to the CENIDE "Mission and Vision". Everyone thinks they know for themselves which strategies and goals they are pursuing together. However, if these thoughts are to be written down, many small differences reveal themselves. But – mission (literally) accomplished! The central message of our common vision is the international visibility for cutting edge materials research and development.

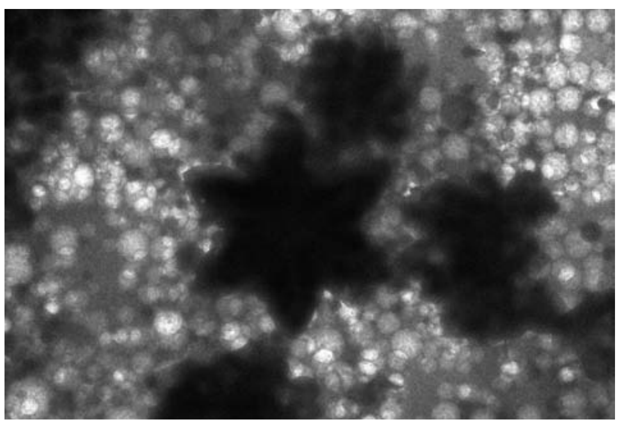
With this in mind, the Scientific Board has identified several main issues that will be addressed in small groups in the future. Although we will contact you about this again in more detail, we would already like to invite you to actively participate in this process.

And now we hope you enjoy reading, browsing and thumbing through!









DEEPER INSIGHTS INTO NANOCATALYSIS

It is about nothing less than putting molecular processes together to form an overall picture. Only by collaborating in different disciplines we can succeed in understanding the basics of heterogeneous catalysis.

Catalysis plays an important role in the chemical industry, on the one hand, because more than 80% of all chemical products are made in catalytic processes, and on the other hand for new applications in energy conversion and storage, e.g., in fuel cells. Within CENIDE, the focus is on the synthesis and characterization of highly active, selective and stable nanomaterials for heterogeneous catalysis .

The aim is to understand the mechanisms of interface reactions in nanocatalysis. By the development of structure-function relationships, relevant structural characteristics for high performance catalysts should be identified and selectively synthesized. In collaboration with the fields of chemistry, materials science, surface science, reaction engineering, and theory, this information is being used to develop and validate an understanding of these molecular processes.

The various catalysis research activities in CENIDE comprise two major third-party funded initiatives: The DFG-funded Collaborative Research Center / Transregio (CRC/TRR) 247 "Heterogeneous Oxidation Catalysis in the Liquid Phase" and the BMBF-funded project KontiKat, which aims at establishing a novel contamination-free process chain for clean size-fractionated catalysts based on pulsed laser ablation in liquids. In addition, CENIDE researchers are involved in coordinated catalysis programs such as the priority programs 1613 and 2080 of the DFG.

CRC/TRR 247
HETEROGENEOUS OXIDATION
CATALYSIS IN THE LIQUID PHASE

July 2018 marked the beginning of the CRC/TRR 247 "Heterogeneous Oxidation Catalysis in the Liquid Phase"; its function is to combine catalysis research and nanotechnology. Selective oxidation is one of the most important chemical processes for functionalizing hydrocarbons and many other raw materials. To achieve high selectivity, many processes are often operated at partial conversion, requiring subsequent energy-consuming separation and raw material recycling. There are well-established large-scale industrial oxidation processes in the gas phase, which are regularly optimized, but not many new processes have arisen in recent years; though liquid-phase operation has the potential for new breakthroughs.

The University of Duisburg-Essen, the Ruhr-University Bochum, the MPI für Kohlenforschung, the MPI CEC, and the Fritz Haber Institute are working together to accumulate fundamental knowledge on the catalytic activity of nanostructured transition metal oxides to better understand the active sites and reaction mechanisms of oxidation reactions at the solid-liquid interface. This knowledge can be used to design new superior catalysts for catalytic processes in favorable mild conditions. The materials focus lies on two structure types of mixed transition oxides, namely spinel and perovskite. These can be synthesized with different compositions and morphologies, while their crystal structure remains stable in the form of a solid solution. The same catalysts are investigated in a selection of complementary oxidation reactions by means of experiment and theory within a coordinated comparative study. These reactions will comprise different fields of catalysis: liquid-phase thermal catalysis, electrocatalysis, and photocatalysis.

Electrocatalysis

Within the CRC/TRR 247, an interdisciplinary group of CENIDE researchers addressed the cation substitution in transition-metal oxides to improve electrocatalysts by the optimization of their composition. In a joint project[1], phase-pure spinel-type $CoV_{2-x}Fe_xO_4$ nanoparticles ($0 \leq x \leq 2$) were introduced as a new promising class of bifunctional catalysts for the oxygen evolution (OER) and oxygen reduction reactions (ORR) due to their high catalytic activity, facile synthesis and low costs. The optimized catalyst in alkaline electrolyte was $CoV_{1.5}Fe_{0.5}O_4$.Theoretical calculations on cation ordering confirm a tendency toward the inverse spinel structure with increasing Fe concentration in $CoV_{2-x}Fe_xO_4$ that already starts

High catalytic activity, facile synthesis and low costs

to dominate at low Fe contents. Contributions to these results came from the CENIDE groups of Heiko Wende (Physics), Stephan Schulz and the newly appointed UA Ruhr Professor for Materials Chemistry of Catalysts Malte Behrens (both Chemistry). Furthermore, the group of Robert Schlögl (MPI CEC), which is also involved in the CRC/TRR, contributed high-end analytics. The calculations were done by the group of Rossitza Pentcheva (Physics).

Her group has additionally published a follow-up work[2] on mixed spinel catalysts in OER with more details of the theoretical modelling: Density functional theory (DFT+U) calculations provide new atomistic insight into the role of surface orientation, termination and composition on the OER activity at mixed $Co_{1-x}Ni_xFe_2O_4$ spinel surfaces. $Co_{1-x}Ni_xFe_2O_4(001)$ (x=0.5, and 0.0) with an additional tetrahedral iron layer (A-layer) and a Co reaction site demonstrates one of the lowest reported overpotentials. Formation of a hydrogen bond of the *OOH intermediate was found at the A-layer which lowers the energy of this rate limiting step.

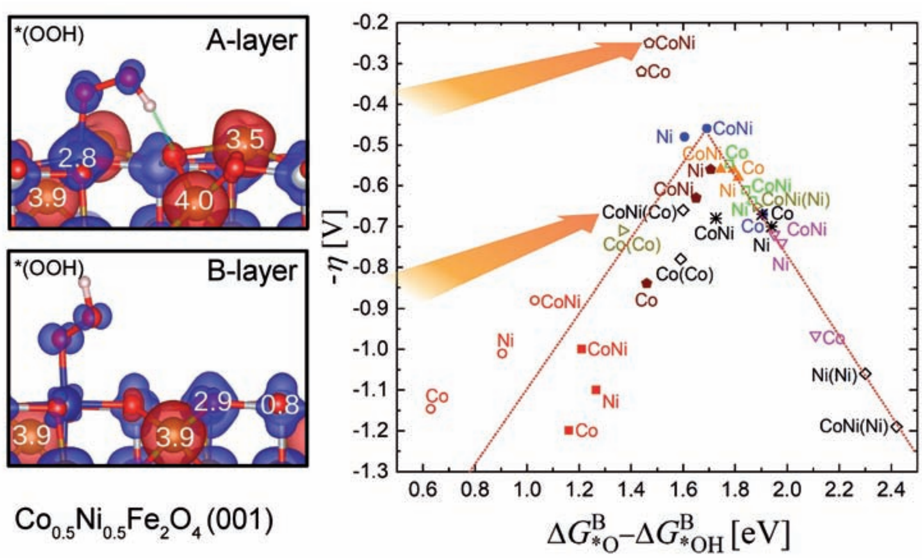


Fig. 1: Overpotential versus the binding energy difference for different reaction sites and terminations of the CoxNi1–xFe2O4 (001) and (111) surfaces (open and filled symbols, respectively).[2]

In a related collaborative work[3] on the spinel electrocatalysts, the groups of CENIDE researcher Stephan Schulz and the 2018 Hellmuth Fischer medallist Kristina Tschulik (Ruhr-University Bochum) investigated the intrinsic catalytic properties of single 4 nm sized cobalt ferrite nanoparticles. They used nano impact electrochemistry to identify the intrinsic electrocatalytic activity of individual nanoparticles and were able to achieve very high current densities as a result of the efficient mass transport. High-resolution transmission electron microscopy and selected area diffraction studies of the catalyst particles confirmed that the particles retain their size and crystal structure even after the harsh OER conditions. This new insight is a key to the efficient development of improved and precious metal-free catalysts for future renewable energy technologies.

The other prototype material of the CRC/TRR 247, noble-metal free mixed perovskite, was investigated in a joint work[4] of the CENIDE groups of Christof Schulz (Engineering) and the newly appointed professor Corina Andronescu (Chemistry) with the groups of Martin Muhler and the 2019 Giulio Milazzo-medallist Wolfgang Schuhmann (both Ruhr-University Bochum). They report the synthesis of $LaCo_{1-x}Fe_xO_3$ perovskite materials by a specifically optimized spray-flame nanoparticle synthesis method using different compositions. An increased Fe content in the precursor mixture leads to a decrease in the electrocatalytic activity of the nanoparticles. For ethanol oxidation, *operando* electrochemistry/ATR-IR spectroscopy results reveal that acetate and acetaldehyde are the final products depending on the catalyst composition as well as on the applied potential.

In the KontiKat project, ligand-free Pt nanoparticles were prepared by pulsed laser ablation in liquids and employed as a benchmarking catalyst to evaluate the durability of a new gas-phase synthesized graphene support in oxygen reduction conditions. This work[5] was conducted as a CENIDE collaboration between the Technical Chemistry I and Institute for Combustion and Gas Dynamics. Raman measurements showed that the graphene was almost defect free. Transmission electron microscopy and initial electrochemically active surface area measurements confirmed good Pt nanoparticle dispersion of the catalysts on both supports. Compared to the commercial catalyst that lost more than 60% of its active surface during harsh aging conditions, the new catalyst retained 95% of its surface area due to a better resistance against carbon corrosion. In another collaboration , the researchers of the Technical Chemistry I and the "The hydrogen and fuel cell center ZBT GmbH" tested these laser-synthesized nanoparticles in a Proton Exchange Membrane Fuel Cell under realistic conditions. A higher catalyst stability and activity of the Pt nanoparticles was found in comparison to a commercially available reference catalyst. Both studies were honoured with the CENIDE best cooperation award of 2018.

The group of Matthias Epple (Chemistry) showed how the porous particle superstructures of electrocatalysts can be visualized by high-angle annular dark-field electron tomography with a resolution of about 20 nm. The catalyst consists of ultrasmall nanoparticles of iridium and iridium dioxide and was prepared by a reduction of sodium hexachloridoiridate with sodium citrate/sodium borohydride in water. Three-dimensional organization of the primary nanoparticles inside a spherical superstructure leads to a high inner porosity of the superstructure and to a pronounced catalytic activity in the oxygen evolution reaction.

Photoelectrocatalysis

The beneficial effects of Sn(IV) as a dopant in ultrathin hematite (α-Fe_2O_3) photoanodes for water oxidation were examined by the group of Rossitza Pentcheva (Physics) in a collaboration[7] with the LMU Munich in the DFG priority program 1613. Combined data from spectrophotometry and intensity-modulated photocurrent spectroscopy yields the individual process efficiencies for light harvesting, charge separation, and transfer. The best performing photoanodes are Sn-doped both on the surface and in the subsurface region and benefit from enhanced charge separation and transfer. The (0001) and (1126)

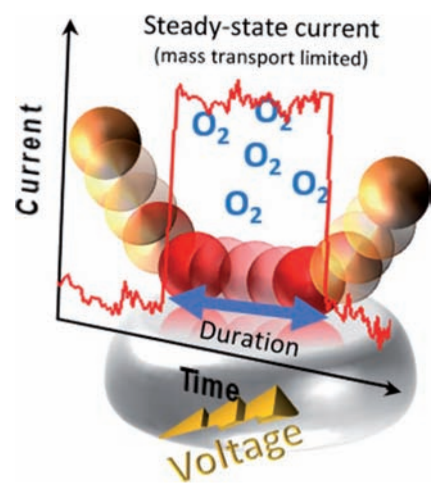


Fig. 2: Nanoparticle OER impact illustration with steady-state current and duration.[3]

terminations of Fe_2O_3 were investigated by DFT calculations. The energetics of surface intermediates during the OER reveal that while Sn-doping decreases the overpotential on the (0001) surface, the Fe_2O_3 (1126) orientation shows one of the lowest overpotentials reported for hematite so far. Electronic structure calculations demonstrate that Sn-doping on the surface also enhances the charge transfer efficiency by eliminating the surface hole trap states and that subsurface Sn-doping introduces a gradient of the band edges that reinforces the band bending at the semiconductor/electrolyte interface and thus boosts charge separation.

A collaboration[9] between the group of Stephan Barcikowski (Chemistry) with the California Institute of Technology showed that laser processing of neat and gold-nanoparticle-functionalized ZnO and TiO_2 nanoparticles enables control of photocurrent generation under simulated sunlight irradiation in neutral aqueous electrolytes. The photoelectrochemical performance of TiO_2 nanoparticles was enhanced more than 2-fold upon irradiation by picosecond−532 nm pulses that healed defects. Laser processing and gold nanoparticle functionalization resulted in colour changes that did not originate from optical bandgaps or crystal structures. Two-dimensional photoluminescence data allowed differentiating and quantification of surface and bulk defects that play a critical yet often-underappreciated role for photoelectrochemical performance as sites for detrimental carrier recombination. The study sheds light on the mechanism of surface and bulk defect generation as a function of laser processing parameters and the effect on the photocurrent. The controlled healing of defects by pulsed-laser processing may be useful in the future design of solar fuels materials.

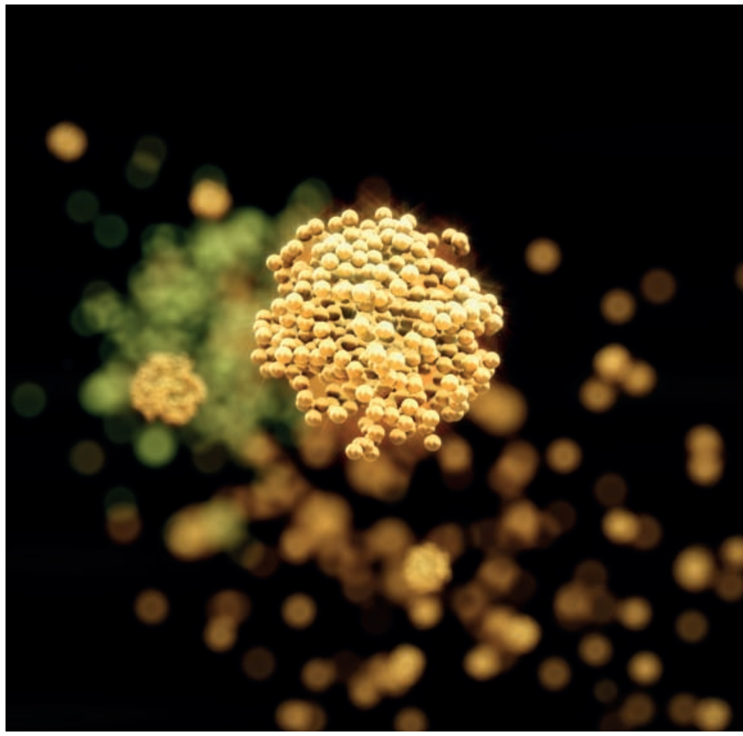


Fig. 3: Laser-based generation of ultra-small particles with countable amounts of atoms. The laser-based production of ultra-small particles with diameters < 3 nm is relevant for biological and catalytic applications as it provides nanoparticles with a unique surface chemistry in the absence of organic ligands.

Thermal Catalysis

In a CRC/TRR 247 collaboration between the CENIDE groups of Stephan Schulz and Rossitza Pentcheva with Martin Muhler and Beatriz Roldan Cuenya (Fritz Haber Institute), crystalline Co_3O_4 nanoparticles with a uniform size of 9 nm were synthesized and applied in the oxidation of 2-propanol after calcination. The high catalytic activity of Co_3O_4 reaching nearly full conversion with 100% selectivity to acetone at 430 K was attributed to the high amount of active Co^{3+} species at the catalyst surface as well as surface-bound reactive oxygen species. DFT+U calculations support the identification of the 5-fold-coordinated octahedral surface Co^{3+} as the active site, and oxidative dehydrogenation involving adsorbed atomic oxygen was found to be the energetically most favored pathway.

Further investigations[10] focused on mixed perovskite oxides, the application of which in selective oxidation reactions in the liquid phase has been rarely studied. Together with the group of Martin Muhler, Christof Schulz and co-workers reported the liquid-phase oxidation of cinnamyl alcohol over spray-flame synthesized $LaCo_{1-x}Fe_xO_3$ perovskite nanoparticles with *tert*-butyl hydroperoxide (TBHP) as the oxidizing agent under mild reaction conditions. $LaCo_{0.8}Fe_{0.2}O_3$ showed the best catalytic properties, indicating a synergistic effect between Co and Fe. The catalysts were found to be stable against metal leaching. The kinetic studies revealed a complex reaction network.

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PANTA RHEI – EVERYTHING FLOWS

At first glance, solid matter seems to be unchangeable. However, the atoms and electrons it contains can be excited from a ground state into a state of higher energy. We aim to develop a microscopic understanding of such non-equilibrium states across materials.

What the Greek philosopher Heraclitus already knew and expressed with this legendary piece of foundational wisdom is: “panta rhei” – everything is in a state of flux. And indeed, this seems to be the nature of our universe where in fact nothing is static. Of course, sometimes things appear to us to be static, because they evolve with an infinite slowness to our human senses that along with the brevity of our lifespans, make us totally incapable of discerning events, as the birth of a planet or the weathering of a mountain range for example. Equally impossible for us to follow in time are all things evolving at inconceivably high speeds, as e.g. the chemical reaction taking place at the membrane of a cell or the movement of an electron around the core of an atom. Our human senses are just not equipped to follow processes which take place on such short time scales. Similarly, we have no natural sense for capturing scales of measurement which lie beyond our own experience, i.e. outside of the range of, let us say, millimetres to kilometres.

However, biological, chemical, and physical processes usually take place on much shorter length and time scales. In order to understand those processes in detail, it is therefore absolutely necessary to look into them more closely, i.e. with high spatial and temporal resolution. This, in turn, is also the key to designing and implementing important applications in the fields of biology, chemistry, physics, and medicine, as e.g. catalysis, electronics, or drug development. If, for example, you knew only the initial and final states of a given system, but had no idea how the system evolved in the interim, how could you hope to understand, not to mention control or optimize the process to suit your needs? This is the reason why CENIDE researchers within the Collaborative Research Centre 1242 “Non-Equilibrium Dynamics of Condensed Matter in the Time Domain” undertake great efforts to achieve a material specific, microscopic understanding of non-equilibrium states and their evolution in time.

Quadrillionth part of a second

Tracking the fraction of an instant

For a long time predominantly static methods with either insufficient or even without any temporal resolution have been used in physics and chemistry, but recently tremendous progress has been made – also due to significant contributions from UDE scientists – with respect to the development of new methods (see info box) capable of taking that closer look. Nowadays, we can follow processes with time-steps as short as femtoseconds (the quadrillionth part of a second, a time span within which even light travels only hundreds of microns) and at atomic length scales. To conduct experiments with such ultra-high precision it is often necessary to specifically prepare the material to be investigated and/or to bring it into an excited, non-equilibrium state by tailored external stimuli, such as light, pressure, electrical voltage, or particles, and this is an art (and science) in its own right. It is this interface between basic research, material science, and method development, at which researchers from CENIDE are working together with colleagues from institutes and universities around the world to actually take that closer look.

Two-dimensional materials provide a very interesting playground for studying such non-equilibrium dynamics. Several groups have conducted experiments on these ultrathin samples which are made up from only a few down to the extreme case of only one layer of atoms (see info box). The group of Uwe Bovensiepen e.g. uses 1T-TaS_2 as a model system to investigate excitations and their dynamics of a Mott insulator. The material exhibits a commensurate charge density wave phase forming a Mott-insulating ground state at low temperature. Population of a single site by two electrons are termed a Doublon. Its formation requires due to Coulomb repulsion the excess energy U. Formation and decay is considered to occur at a rate J if an adjacent hole (here a holon) is available. Using femtosecond time-resolved photoelectron spectroscopy the researchers together with colleagues from Fribourg (Switzerland), Kiel, and Hamburg (both Germany) could identify the Doublon at an energy just below 200 meV above the Fermi level of the metallic high temperature state. They found in addition that the relaxation time of the Doublon is shorter than the available temporal resolution, but in agreement with a limit determined by the simple estimate $\hbar/J$. They also observed a continuum of electronic excitations at higher energy which are assigned to the population of unoccupied Bloch bands and – interestingly – do not repopulate the Doublon state. This can be understood by formation of a bottleneck since excitations at energies smaller than the Doublon formation energy are inhibited by the insulating character of the Mott state.[1]

Graphene – Another amazing property discovered

Another example of the exciting properties of 2D materials is the work of Dmitry Turchinovitch (former UDE, now at University of Bielefeld) who, together with his co-workers from Helmholtz Zentrum Dresden Rossendorf, demonstrated that

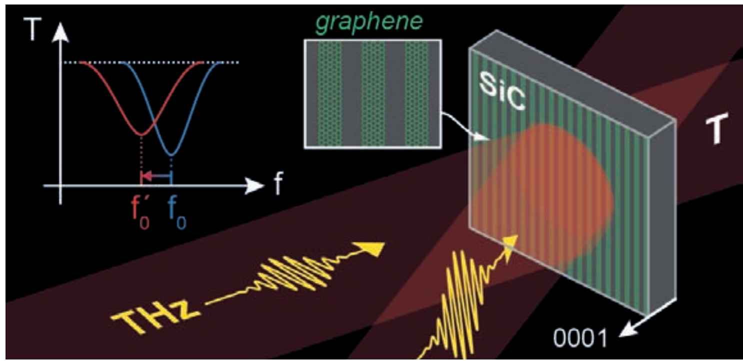

Fig. 1: Employment of nonlinear pump–probe measurements on subwavelength graphene ribbons to explore the effect of photoinduced hot carriers on graphene plasmons. Measurements taken above and below the plasmon resonance frequency demonstrate an optically induced red-shift of the plasmon resonance, which is a signature of hot carriers in graphene. (Reprinted with permission from M.M. Jadidi et al.: Optical Control of Plasmonic Hot Carriers in Graphene. ACS Photonics 6, 302-307, 2019. Copyright 2019 American Chemical Society.)[3]

Pump-probe-experiments

One important tool for researchers to obtain experimental data with ultra-high time resolution is the so-called pump-probe technique. At time zero, the system under investigation is excited via an ultra-short and intense laser pulse. The system will relax back into its ground state within a given time. Before that happens, after some predefined waiting time ("delay"), the system´s transient state is probed by a second ultra-short (usually weaker) laser pulse, e.g., by measuring its optical absorption. This is repeated with systematically increasing delays between excitation and probe pulse. In this way snap-shots of the transient states during relaxation can be taken, separated by time-steps which are limited only by the duration of the pump/probe pulses. Stitched together the snap-shots represent a movie of the dynamics. The Nobel Prize in Physics 2018 was awarded to Gérard Morou and Donna Strickland for developing "their method of generating high-intensity and ultra-short optical pulses" which are the key element for pump-probe-experiments.

graphene has (yet another) unique property. Graphene, the two-dimensional hexagonal lattice of carbon atoms, stands out amongst other materials because of its mechanical strength, good heat conductance and its high electron mobility. The latter means that electrons in graphene can be easily accelerated by electromagnetic fields. The scientists exploited this to multiply the frequency of the outer field they applied: Instead of the initial frequency of one Gigahertz (one billion oscillations per second), they found that the accelerated electrons oscillated with a frequency which was higher by a factor of thousand (Terahertz). This effect had been predicted in theory and was now nicely confirmed by the experimentalists. It can be used for novel, ultrafast transistors with extremely high clock rates.[2]

The same material system was investigated by Martin Mittendorff (newly appointed Professor at UDE, PI CRC 1242). Graphene´s band structure allows interband ex-

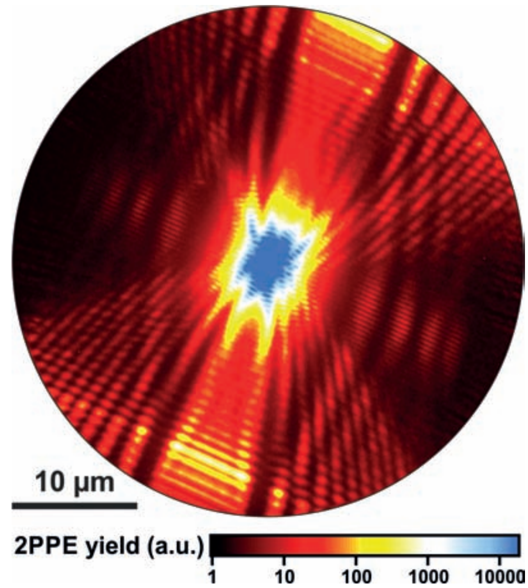

Fig. 2: Focus point of a surface plasmon polariton wave that is formed by two Fresnel-type grating couplers. Such grating couplers, visible at the lower left and the upper right of the image, excite plasmon waves only at distinct areas on the surface, so that the interference pattern of the excited waves forms a focus point. In the focus, the electric field of the surface plasmon polariton is so strong that electrons are emitted from the focus by a nonlinear mechanism.[6]

Two-dimensional solids

Solids in physics are often idealized as single crystals, i.e. atoms fixed in space to positions forming an ordered array in all three directions. Such a three-dimensional system can be investigated by experimentalists with high accuracy, theoreticians can easily treat it exploiting the symmetry, and the number of material systems showing interesting properties such as superconductivity, magnetism, or shape memory seems endless. Yet, in 2004, two scientists managed to add yet another class of exciting materials to solid-state physics by reducing such a three-dimensional solid to two dimensions: They succeeded in peeling a single layer of carbon atoms from a graphite crystal with a piece of 3M tape. The result was not only the thinnest solid ever fabricated it also turned out to have many intriguing properties not found in its 3D counterpart. Graphene, the first 2D material to be discovered, has a mechanical strength comparable to diamond and conducts current better than silver. Those record values motivated researchers to look for other 2D materials and in the meantime dozens have been fabricated with no end in sight. The Nobel Prize in Physics 2010 was awarded to Andre Geim and Konstantin Novoselov "for groundbreaking experiments regarding the two-dimensional material graphene".

citation of electrons in a wide spectral range and the high charge carrier mobility enables the fabrication of very efficient plasmonic devices based on graphene, strongly enhancing the light-matter interaction at the plasmon frequency. While the nonlinear optical properties of graphene had already been exploited for applications, e.g. as saturable absorbers in mode-locked lasers, the enhanced nonlinearity of plasmonic absorption remained for the most part unexplored. The Mittendorff group, together with his co-workers from the US (Maryland) and Dresden, used an interesting technique to get a closer look: They tuned the plasmon frequency of the material by cutting graphene into small ribbons. Pump-probe experiments on theses samples showed that graphene ribbons reveal strong enhancement (more than two orders of magnitude) of optical nonlinearity compared to unpatterned graphene. The experimental results are in excellent agreement with theoretical calculations based on a hot-carrier model: as the carriers absorb the pump pulse their temperature increase which results in a decreased chemical potential, causing the plasmons to shift to lower frequencies. While in most materials thermal nonlinearities are inherently slow, the fast carrier cooling in graphene leads to ultrafast redshift of the plasmon frequency, which can be exploited in THz nonlinear devices like optical switches.[3]

Data storage with new phase change materials
Switching is also something, Klaus Sokolowski-Tinten (PI CRC 1242, CENIDE member) took a closer look at. He investigated the atomic processes taking place in so-called phase change materials (PCMs). These materials have been used for quite some time in rewritable CDs and other optical storage media, but nowadays find ever increasing application in electronic memory with the ultimate goal of realizing universal storage media that are fast (as RAM) and non-volatile (as FLASH) at the same time. When PCMs are heated by an electrical or optical pulse, they change from a glassy to a crystalline state, and vice versa. These two different states represent the '0' and '1' of the binary code needed to store information. While this switching had already been discovered in the 1990s and is thus well established from an engineering point of view, nobody knew how it really worked on an atomic scale. By using time-resolved X-ray diffraction after melting the PCM with a short laser pulse Sokolowski-Tinten together with his colleagues from Germany, the US, Sweden, Switzerland, and Spain could follow the transition from the liquid to the glassy state in time and space, resolving the underlying structural transformation with femtosecond resolution. They found that when the liquid is cooled sufficiently far below the melting temperature, it undergoes a structural change to form another, low-temperature liquid phase. While the high temperature liquid is rather metallic and can therefore crystallize very quickly to produce the "on" state, the newly discovered low temperature phase has more rigid chemical bonds, which helps to stabilize the glassy "off" state at ambient conditions. These results represent an important step towards optimized PCM-based memory devices.[4]

Super slow motion on the femtosecond scale
A clever sample design in combination with ultra-high time resolution is also the key to the work of Frank-J. Meyer zu Heringdorf (PI CRC 1242, CENIDE member). He applied the concept of a so-called zone plate, originally invented by Jean Fresnel (who also developed the Fresnel lenses used in lighthouses) already in the 19th century. The plate is basically a hologram that uses diffraction to form a defined focal point when it is illuminated with a planar light wave. The team around Meyer zu Heringdorf applied this to surface plasmon

Imaged in super slow motion

polaritons (SPPs), i.e. electron density waves that propagate at metal surfaces at almost the speed of light. Instead of using a zone plate to focus propagating plasmon waves, however, the team developed a suitable Fresnel excitation structure that directly and effectively converts light into plasmon waves with the appropriate properties to form a focal point. Using time-resolved photoemission electron microscopy under normal incidence for imaging SPPs at their native wavelength, a technique introduced by the team in 2018, the "Fresnel optics for surface plasmons" could be precisely characterized and the formation of the focal point of the plasmon waves could be imaged in super slow motion on the femtosecond scale.[5,6]

These are just a few examples highlighting the results obtained within the CRC 1242 which has been running for almost four years now. As with everything else, the CRC 1242 is not itself a static system but evolves with time. Within the next funding period researchers plan to go yet another step further and shift their focus from observing more towards *controlling* the dynamics of the processes they are interested in. By addressing these new challenges, CENIDE researchers will surely make more exciting discoveries in the field of non-equilibrium dynamics in the years to come.

CRC 1242
The dynamics of elementary excitations in solids, on surfaces or in nanoparticles or nanostructures are being investigated with the highest time resolution: Structural excitations, phase transitions, transient heating and cooling are traced with electron or X-ray diffraction with time resolutions of a few 100 femtoseconds. The even faster dynamics of the electron system are being investigated using photoelectron emission spectroscopy or microscopy with a time resolution of only 10–20 femtoseconds. With the help of these methods, numerous new discoveries about mechanisms on the nano-scale are being made.

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UNDERSTANDING SYNTHESIS TO THE DETAIL

The size of our nanomaterials synthesis plants range from the laboratory to the pilot-plant scale. This combination allows for the thorough examination of underlying processes – and for building demonstrators based on substantial amounts of nanomaterials in various application field.

Gas-phase synthesis of functional nanoparticles is a long-standing focus area of CENIDE. The work ranges from understanding the fundamentals to the development of processes that are scalable to industrial production. Experimental work, modeling, and simulation are closely interlinked with the aim to generate a comprehensive understanding of the processes that often occur in multiple phases on a wide range of time scales and spatial dimensions.

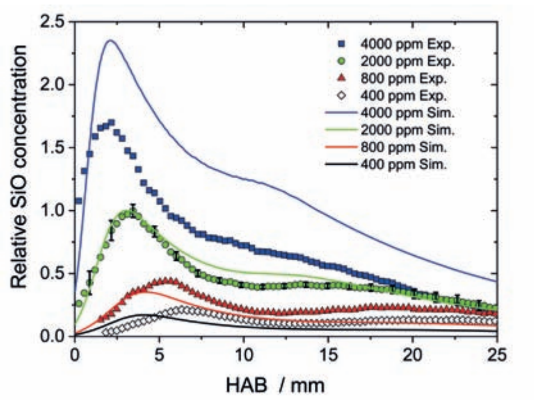
Synthesis of complex nanostructured materials from gaseous and evaporated precursors

The DFG Research Unit FOR 2284 is devoted to the synthesis of complex nanostructured materials from gaseous and evaporated precursors. The materials' complexity arises from the fact that the resulting materials should not only be well defined in composition, primary particle size, and crystal structure. They should also have defined secondary and tertiary structures such as core-shell, aggregates with defined and variable porosity and surface decoration that are all derived from specific applications that are mainly connected with CENIDE's priority areas in "Nanotechnology in technical applications" (i.e., batteries, thermoelectrics, photovoltaics) and "Catalysis".

To correctly describe nanoparticle synthesis from gas-phase precursors, as a first step, it is important to understand the mechanism and kinetics of the initial reactions of the precursor. This has been studied with microsecond time-resolution in shock-tube experiments in Mustapha Fikri's group for the thermal decomposition of tetramethyl-silane[1] and for the reaction of tetramethoxy-silane with hydrogen atoms.[2] Such experiments lay the foundation for the development of detailed reaction mechanisms for the initial reactions in the gas-phase. Systematic comparative experiments of precursors carrying the same central element (here silicon) with variable chemical ligands, will lead to an understanding of the structure-reactivity relationships using theoretical concepts such as the group additivity method.[3]

A critical check for the validity of reaction mechanisms is provided by species-resolved measurements in laminar flames with novel laser-based methods in Thomas Dreier's group. This has been done for quantitative imaging detection of silicon monoxide[4] and the temperature distribution in the reaction zone where precursors decompose and first particles form. In a combined work of experiment and simulation (Irenäus Wlokas's and Andreas Kempf's groups), synthesis of SiO_2 nanoparticles in flames was investigated.[5] Unexpected experimental results concerning the spatial distribution of the intermediately formed SiO indicated that $(SiO)_n$ clusters are intermittendly formed – a significant step towards a better understanding of the formation of this material in flames (Figure 1).

Controlling the oxidation state of iron and the crystal structure of iron containing compounds is key to generating materials with well defined properties such as iron oxide nanoparticles for cancer treatment or heterogeneous catalysis. Iron oxides contain iron in different oxidation states and form different phases for one valence state are being investigated in Markus Winterer's group. It was shown that gas-phase synthesis enables the reproducible production of pure nanocrystals with narrow size distributions.[6] The dependence of



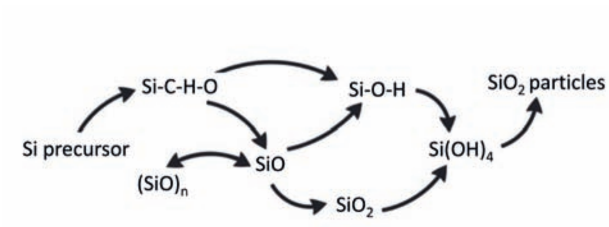


Fig. 1: Spatial distribution of the intermediately formed SiO in the flame-synthesis of SiO_2 along the flow direction behind the flame (HAB). The "dip" in the concentration profiles indicated that there is – in contrast to previous understanding – an initial loss path for SiO at intermediate temperature that leads to the formation of $(SiO)_n$ clusters that then partially evaporate and further oxidize towards product SiO_2 formation.

particle characteristics such as size, specific surface area, degree of agglomeration or crystallinity on the process parameters – especially the time-temperature-profile in gas-phase synthesis – has been investigated in detail in Markus Winterer's group.[7]

Spray-flame based synthesis

As an alternative to using gaseous precursors, the members of the DFG Priority Program SPP 1980 investigate spray-flame based synthesis methods, especially for generating multinary oxides that also play an important role in the context of catalysis in the CRC/TRR 247. As a basis for the coordinated research within the SPP, CENIDE researchers have developed a standard experiment, the SpraySyn Burner[8] that has now been distributed to around 20 laboratories not only in Germany but also in China and the US. The investigation of the spray-flame synthesis of nanoparticles at a well-defined standard burner by experiment and simulation now makes it possible to produce a comprehensive data set with various established and novel measuring methods.

For catalysis applications, noble-metal-free perovskite nanoparticles have successfully been synthesized in Hartmut Wiggers's group. The influence of the choice of solvents on the spray-flame synthesis of $LaFeO_3$ and $LaCoO_3$ perovskites on chemical reactions in the solution, the product composition, phase purity, morphology, and the electrocatalytic activity was clarified.[9] To this end, metal nitrate precursors were dissolved in pure ethanol and in ethanol/2-ethylhexanoic acid mixtures and processed in the spray flame. While experiments with ethanol led to a broad particle-size distribution and to the formation of undesired phases such as La_2CoO_4, La_2O_3, and Co_3O_4, the addition of 2-EHA led to the formation of single-phase, high-surface-area $LaCoO_3$ perovskite nanoparticles with a narrow size distribution.

$LaCo_{1-x}FexO_3$ perovskites have also been successfully synthesized in sprayflames. Structural characterization of the resulting materials by XRD, TEM, FTIR and XPS revealed the formation of mainly perovskite-type materials (Figure 2). The catalytic activity of these materials has been studied in collaboration with Martin Muhler[10] and Wolfgang Schuhmann[11] (Ruhr-University Bochum). The spray-flame synthesis enables a step-wise variation of the elemental composition of the perovskites. An increased Fe content in the precursor mixture was found to lead to a decrease in the electrocatalytic activity of the nanoparticles.

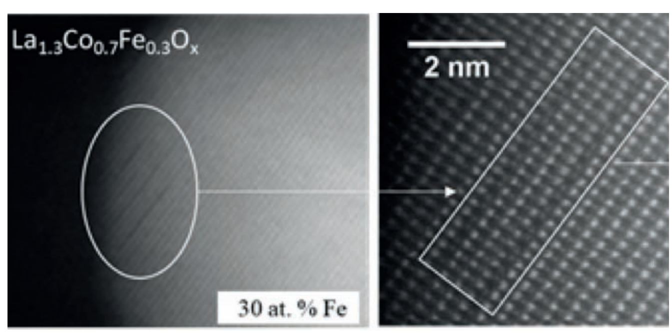


Fig. 2: TEM characterization of spray-flame-synthesized ternary oxides. Here: Ruddlesden-Popper phases.

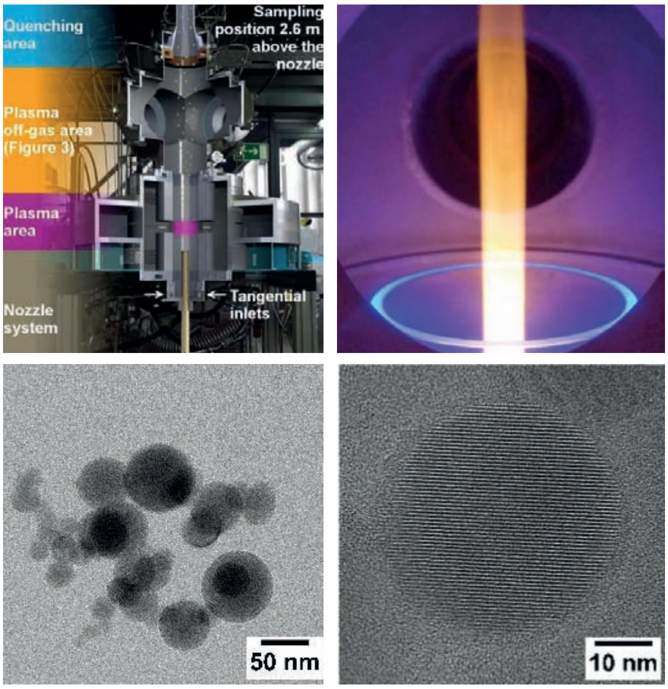


Fig. 3: Microwave plasma synthesis of crystalline silicon nanoparticles in a scaled-up reactor. The flow containing hot particles (orange) is stabilized by a swirling tornado-like gas flow.

Award-winning spin-off

The field of flame synthesis of nanoparticles led to the spinoff of the company HSWmaterials in 2017, which received two awards in 2018 from the city of Kevelaer and the Kleve district.

Plasma synthesis

The scale-up of materials synthesis in gas-phase reactions also plays an important role for the discharge-based generation of metal nanoparticles[12] in a production facility through parallelization of multiple transferred arcs in one reactor was developed by Einar Kruis's group. The synthesis of silicon nanoparticles in a pilot-plant-scale microwave plasma reactor was successfully implemented at IUTA and enables the generation of particles that are relevant, e.g., for application in batteries.[13] It was possible to ensure reproducible, long-term operation of the reactor through gas-dynamic stabilization of the reacting flow and to control particle size and morphology via the gas flow velocity and the precursor concentration (Figure 3).

Plasma synthesis has also been successfully used for the synthesis of substrate-free few-layer graphene from vaporized hydrocarbons[14]. The physico-chemical properties of the resulting material ere characterized and compared with those of reduced graphene oxide (rGO) made by Hummers' method. The results indicate that the gas-phase synthesis method provides highly-ordered few-layer graphene with an extraordinary high purity, very low oxygen content of less than 1 at.%, and high specific conductivity. Both graphene materials were processed towards silicon-graphene nanocomposites for Li-ion battery anodes. Subsequent electrochemical testing revealed that the gas-phase graphene significantly enhances the long-term stability and Coulomb efficiency of the composite compared to pristine silicon and outperforms the composite fabricated from reduced graphene oxide.

The gas-phase synthesized graphene has been successfully decorated with ligand-free platinum nanoparticles generated by laser ablation in the liquid phase by Stephan Barcikowski's group[15]. During durability tests, graphene supported Pt nano-

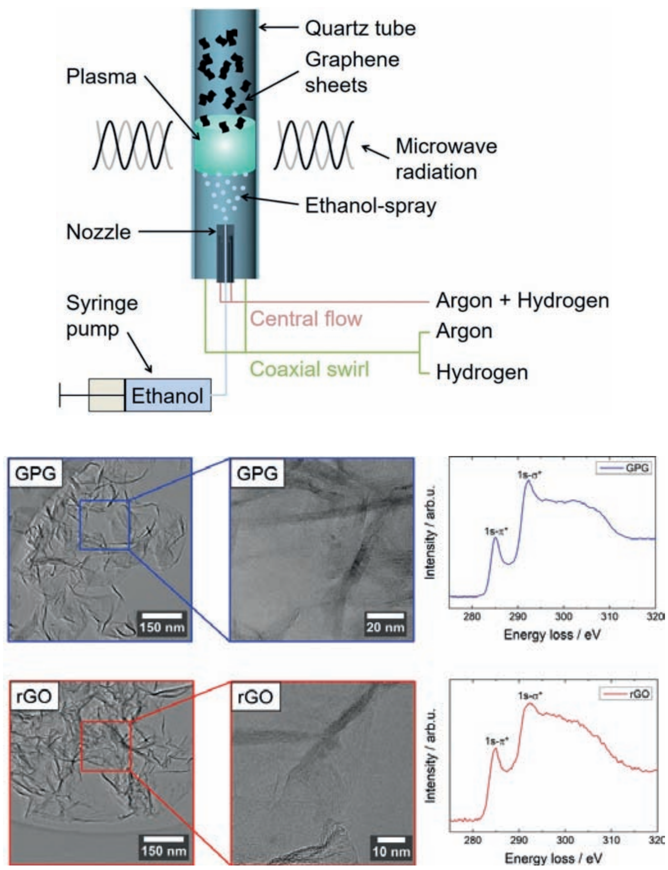
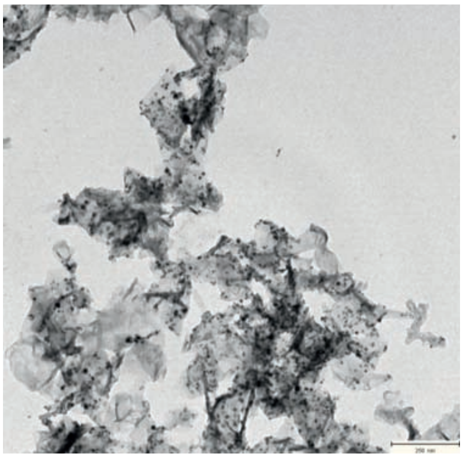


Fig. 4: Graphene synthesis in the lab-scale plasma reactor. Comparison of the gas-phase-synthesized (GPG) graphene and reduced graphene oxide (rGO) based on TEM and EELS measurements.



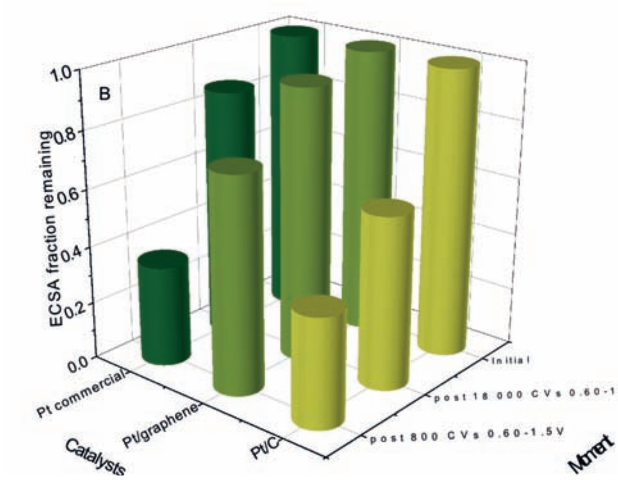


Fig. 5, Left: TEM micrographs of laser-generated Pt NPs on gas-phase synthesized graphene. Right: Improved stability of the graphene supported platinum catalyst: Pt ECSA after the load ADT and after the start/stop ADT protocol for nanoparticles supported on Vulcan, on GPG and for commercial Pt/C (normalized).

particles showed much better ECSA retention, ultimately retaining a higher ECSA than a commercial sample subjected to the same procedure (Figure 5).

Inductively-coupled plasma-enhanced chemical vapor deposition (ICP-PECVD), on the other hand, was shown to lead to the deposition of carbon nanowalls (CNWs) on silicon, stainless steel, nickel and copper substrates from hydrocarbon precursors.[16] The CNWs are electrically conducting and show a large specific surface area, which is a key characteristic in order to make them interesting for sensors, catalytic applications or energy-storage systems.

Diagnostics

Inline and *in situ* diagnostics of particle-generation flows is an important prerequisite towards understanding the underlying processes and validation of simulation methods. A new ejector-based sampling system was developed by Einar Kruis‘s goup, enabling sampling of aerosols from low-pressure environments and their subsequent analysis methods that are only applicable at atmospheric pressure.[17] The vacuum ejector was successfully demonstrated in Hartmut Wiggers‘s group during particle synthesis in a low-pressure microwave plasma reactor with a combination of online instrumentation.

For optical diagnostics, new methods that combine absorption, laser-indcued incandescence and laser-induced breakdown spectroscopy were used to observe the formation of silicon and germanium particles in plasma flows by Christof Schulz‘s and Thomas Dreier‘s groups in collaboration with Kyle. Daun (University of Waterloo).[18] The optical properties of the molten nanoparticles were successfully described by Drude model parameters.

CENIDE’s work on gas-phase synthesis of nanoparticles is gaining international recognition. In September 2018, around 100 experts from academia and industry met in Duisburg for the 3rd international symposium on “Gas-Phase Synthesis of Functional Nanomaterials”. The audience included participants from from China, Israel, Turkey, Switzerland, Great Britain, Finland, the USA, and Australia. A plenary presentation on the 37th international Symposium on Combustion[19] on Gasphase synthesis of nanoparticles by Christof Schulz showcased the advances in fundamental understanding and process understanding that is systematically expanded by the CENIDE team to a large international audience. Through the DFG Mercator Fellowship Program, Kyle Daun (University of Waterloo, Canada), Greg Smallwood (National Research Council, Canada), Igor Rahinov (Open University of Israel), Jay Jeffries (Stanford University, USA), and Sergey Cheskis, University of Tel Aviv, Israel) spent several weeks or even months in Duisburg. Additionally, Markus Kraft (Cambridge University, UK) and Hai Wang (Stanford University, USA) spent significant time in Duisburg related to their prizes awarded by the Alexander von Humboldt Foundation.

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MAGNETIC CONCEPTS FOR COOLING

Developing a fascinating new cooling technology: Magnetocaloric materials require neither ozone-depleting nor hazardous chemicals and are significantly more efficient than the conventional vapour compression refrigeration.

With the increase of the standard of living in emerging countries, e.g., India and China, the demand dramatically rises for energy efficient cooling devices for domestic refrigeration and also for air conditioning. For future devices the conservation of energy and the reduction of greenhouse gas emissions are essential. Currently, new developments for cooling technologies are on the horizon which make use of the magnetic behaviour of solids, representing a fascinating alternative to conventional vapor-compression refrigeration due to the superior efficiency of the magnetocaloric materials and the omittance of ozone depleting or hazardous chemicals and greenhouse gases. It is the vision of a large consortium of scientists at CENIDE in the experimental workgroups of Mehmet Acet, Michael Farle, Katharina Ollefs and Heiko Wende together with Markus Gruner in the theory workgroup of Rossitza Pentcheva from Physics that the use of magnetocaloric materials in new cooling devices provide an energy effective alternative to conventional vapor-compression refrigeration. To advance this field these scientists teamed up with Oliver Gutfleisch at the TU Darmstadt within the project "Novel caloric materials by mastering hysteresis: from basic mechanisms to applications" which was funded by the DFG within the priority programme SPP 1599 "Caloric Effects in Ferroic Materials: New Concepts for Cooling".

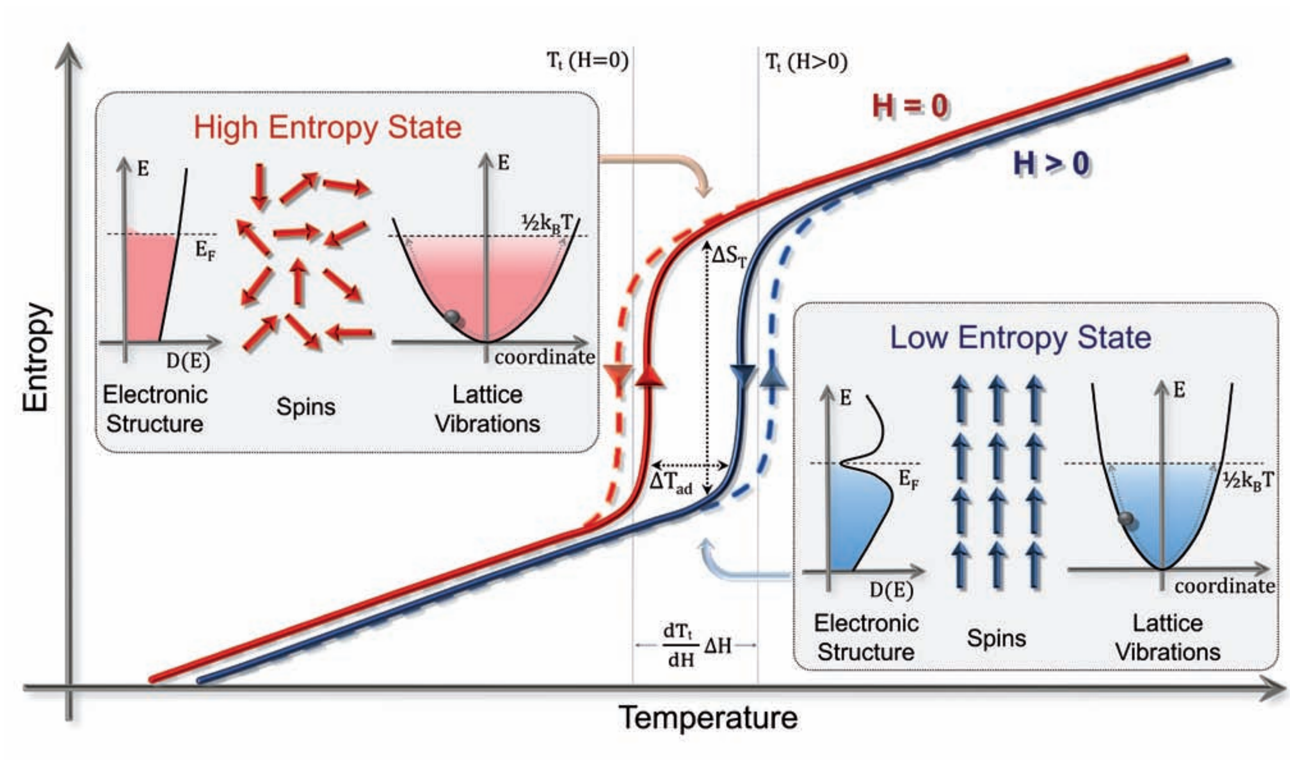
The new research results of this consortium are summarized in a recent review in a Special Issue on "Ferroic Cooling".

New cooling devices provide an energy effective alternative.

In this review the scientists describe how the combination of advanced characterization techniques, e.g., at large scale facilities such as synchrotron radiation sources, with theory provides a fundamental understanding of the magnetocaloric effect in new functional magnetic materials. For cooling purposes, it is important that the application of a magnetic field to a magnetocaloric material is associated with a large change of temperature under adiabatic conditions, or, respectively, a significant change of entropy in an isothermal process. Rapid changes of entropy are found for first-order structural transitions at a specific transition temperature T_t. The application of a magnetic field leads to a shift of the transition temperature without mag-netic field $T_t(H=0)$ to higher temperature $T_t(H>0)$ (Fig. 1).

Thermodynamic cycle with four steps

For a magnetic refrigeration application, a thermodynamic cycle is required with four important steps: 1) A magnetic field



is applied to a magnetocaloric material under adiabatic conditions, i.e., without exchange of heat with the environment, leading to a field-induced structural transition. For a conventional magnetocaloric material the decrease of entropy by the ordering of the magnetic moments (see the ordered arrows depicting the spins in the box on the right in Fig. 1) is then compensated by increasing the temperature of the material. 2) The heat of the material is transported to the hot reservoir of the cooling device. This leads to the warm back of a refrigerator known to anyone familiar with this ubiquitous kitchen appliance. 3) Then the magnetic field is rapidly decreased to zero. This change is carried out again adiabatically, which consequently results in a decrease in the temperature of the magnetocaloric material. 4) Now the cold reservoir (which is the food in the refrigerator) is thermally coupled to the cold magnetocaloric material. In this manner the food is cooled and the magnetocaloric material warms up again to the temperature at step 1). By cycling this process, the food (often a bottle of beer is used as a test system) can be cooled down to the required temperature. As mentioned above, large entropy changes and thereby large adiabatic temperature changes can be achieved at first-order magnetostructural transitions. Here, changes in the structure are accompanied by dramatic modifications of the magnetic order. However, these first-order magnetostructural transitions exhibit thermal hysteresis effects as presented in Fig. 1. The red solid line and the red dashed line (high entropy state) show this thermal hysteresis as it is also the case

Fig. 1: Schematic entropy-temperature diagram illustrating the magnetocaloric effect at a first-order transition. Application of a magnetic field H shifts the transformation temperature T_t to higher values. Applying the magnetic field isothermally in the intermediate temperature range between T_t (H=0) and T_t (H>0) leads to a decrease of ΔS_T in the total entropy, whereas an adiabatic field release decreases the temperature by ΔT_{ad}, which can be used for heat transport or cooling. Thermal hysteresis, indicated by the dashed lines, causes heat dissipation and reduces the maximum possible ΔT_{ad} in a cycling setup. The boxes depict basic characteristics of the respective high- and low-entropy states of the three relevant degrees of freedom. For the electronic entropy, these are, respectively, a high or low density of states at the Fermi level $D(E_F)$, for the magnetic entropy orientational disorder or order of the atomic moments, and for the lattice entropy, the presence of on-average softer or stiffer vibration[1].

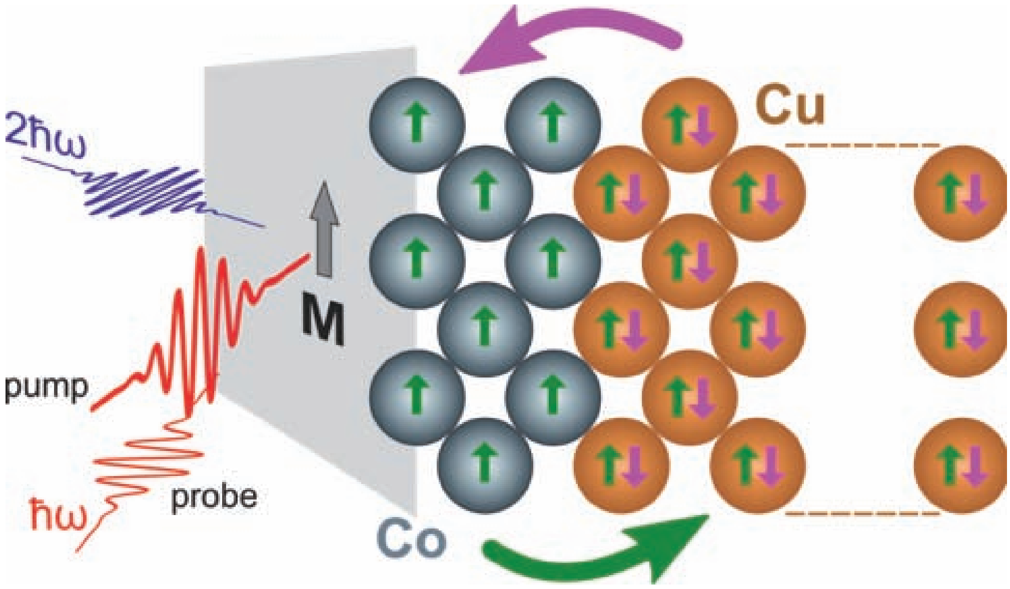


Fig. 2 (Reprinted figure with permission[2]): Illustration of the epitaxial model interface Co/Cu(001), the interface-sensitive pump-probe experiment, and spin transfer dynamics. Vertical arrows indicate spins and ferromagnetic order in Co. Cu carries negligible spin polarization before optical excitation. Horizontal arrows represent spin transfer across the interface. The Co magnetization M is oriented perpendicular to the optical plane.

Bottle of beer is used as test system

for the solid blue line and the dashed blue line (low entropy state). This reduces the size of the reversible adiabatic temperature change ΔT_{ad}. Here a dilemma becomes obvious: On the one hand, a rapid change of the magnetization at a first-order transition is advantageous. On the other hand, the first-order transition comes with a thermal hysteresis which reduces the adiabatic temperature change ΔT_{ad} which can be exploited in a device. This demonstrates the need to master hysteresis for the improvement of magnetocaloric materials. Within the consortium the most promising first-order magnetocaloric materials such as Ni-Mn-based Heusler alloys, FeRh, $La(FeSi)_{13}$-based compounds, Mn_3GaC antiperovskites, and Fe_2P compounds were studied. The CENIDE scientists and their collaborators revealed the microscopic contributions of the entropy change, the magnetic interactions, the effect of hysteresis on the reversible magnetocaloric effect (MCE), and the size- and time-dependence of the MCE at magnetostructural transitions experimentally as well as theoretically.

As an example, Nuclear Resonant Inelastic X-ray Scattering (NRIXS) experiments at synchrotron radiation facilities were combined with density functional theory (DFT) to resolve element- and site-resolved vibrational properties. For the functional magnetocaloric material $La(Fe,Si)_{13}$ the consortium found an unexpected strong red-shift of the vibrational density of states VDOS at T_t. This shift appears although the lattice constant decreases, which is responsible for a significant cooperative vibrational entropy contribution ΔS_{lat} originating from the Fe sites. It is important that thereby the lattice contribution to the entropy change ΔS_{lat} has the same sign as the electronic contribution ΔS_{el} and the magnetic contribution ΔS_{mag}.

This behavior is explained by the itinerant metamagnetism of the Fe atoms, which couples all degrees of freedom.

Taking all the results together, a detailed understanding of important mechanisms was achieved that has significant impact on the performance and hysteresis of magnetocaloric materials. In future studies the consortium plans to identify all relevant intrinsic and extrinsic sources of hysteresis, their microscopic origins, and entanglement on various length and time scales. The CENIDE scientists are confident that the thorough description of these properties will lead the discovery of new efficient magnetic energy conversion materials which will be utilized in future cooling applications. For these applications it is expected that magnetocaloric materials with the mass of several kilograms will be used in a refrigerator.

Quantum dynamics in tailored intense fields

A completely different route for the use of magnetic materials with unusual properties is pursued in the DFG funded project in the priority program SPP 1840 "Quantum Dynamics in Tailored Intense Fields" (QUTIF) by Andrea Eschenlohr in the workgroup of Uwe Bovensiepen at the Faculty of Physics in collaboration with the theoretical physicist Sangeeta Sharma and collaborators in the group of Eberhard Gross at the Max Planck Institute of Microstructure Physics in Halle: Ultrafast magnetic phenomena are studied for magnetic films with a thickness of few atomic layers only.[2] These ultrathin systems have the potential for new electronic devices that make use of the magnetic moment of the electrons which is connected to the spin. This field is therefore called spintronics. Because of the need to establish very fast switching behavior in these devices, the advancement of the fundamental understanding of ultrafast magnetization dynamics including femtosecond spin injection is necessary to control the spin-response on a microscopic level.

This has been achieved by Andrea Eschenlohr and collaborators by excitation of ferromagnetic/paramagnetic metallic heterostructures with ultrashort laser pulses. They unraveled the microscopic processes behind optically excited spin dynamics at the model interface of an ultrathin epitaxial Co film on a Cu single crystal (Co/Cu(001)) by combining femtosecond time-resolved interface-sensitive nonlinear magneto-optical experiments and ab *initio* time-dependent density functional theory. The CENIDE scientists and their collaborators have found that spin-dependent charge transfer between Co and Cu dominates the initial magnetization dynamics as schematically presented in Fig. 2. Interestingly, this includes a contribution from resonantly enhanced minority spin transfer from Cu to Co (magenta arrows in Fig. 2) due to electronic hybridization

Control the spin-response on a microscopic level

at the interface, which indicates new possibilities for controlling femtosecond spin dynamics via tunable laser pulses and/or engineered interface properties. Moreover, ultrafast spin transfer competes with a loss of spin polarization by spin flips already mediated through spin-orbit coupling on sub 100 fs timescales, which ultimately limits the spin injection efficiency.

The two examples demonstrate that the advancement of a fundamental understanding of magnetic materials paves the way toward new and fascinating applications in different fields of efficient energy conversion and spintronics.

In the field of magnetic materials, the focus at CENIDE in general is on the production and highly specific characterization of new materials and hybrids from the microscopic to the macroscopic length scales and on ab-initio modelling. Both ultra-thin metallic and oxidic films, nanoparticles as well as molecular nanomagnets play an important role as building blocks for modern hybrid systems. In terms of characterization, the analysis of the high-resolution spin-polarized electronic structure, spin structure and spin texture, spin-dependent transport and spin dynamic up to that of ultra-short time phenomena is crucial. The integration of fundamental research and material research with high potential for application provides the basis for close collaboration of the university's groups with industry.

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INTERACTING WITH BIOLOGICAL SYSTEMS

From destroying pathogens and cancer cells to the formation of self-evolving structures.

Biomaterials are natural or artificial substances in contact with biological systems. CENIDE is involved in the investigation of this interaction between materials, surfaces, particles, and macromolecules. The research area benefits from expertise in material science and bioscience and the chemically or physically orientated sciences – for example, in the exciting field of nanobio photonics.

First of all, we welcome our new colleagues, Lawrence Livermore engineer Brian Giera and our new collaboration partner Stephan Link (Rice University/USA), both of whom have been awarded with Mercator Fellowships by the DFG. Brian Giera has recently begun a three-year visiting professorship at the University of Duisburg-Essen. In collaboration with Barcikowski he will be developing a method for uniformly coating neural implants with biocompatible metallic nanoparticles, adding his computational expertise, in particular, to nanoparticle-based simulation of electrophoretic deposition (EPD) for the coating of objects with materials using electrical fields. Stephan Link, internationally recognized for his work on single-particle spectroscopy in plasmonics, will support Stephan Barcikowski's work in destroying multi-resistant pathogens (MRE) with so-called guided nanorockets, equipped with drugs which have the great advantage of releasing nanosilver in place and thus destroying the bacteria. MRE has led to thousands of complications, sometimes life-threatening, in German hospitals every year. No one who becomes infected after implantation is susceptible to antibiotics. The challenge is to create nanoparticles which dissolve at the right time and place, i.e., only where the anti-microbial silver meets the pathogens, thus preventing the destruction of cell tissue. In addition, with its expertise in the preparation of biocompatible nanoparticles, Stephan Barcikowski‘s research group is a project partner of the new Research Training Group within the University Alliance Ruhr (UA Ruhr) "Precision Particle Therapy – Applied Physics and Chemistry at the Interface with Medicine", which will be funded by the Mercator Research Center Ruhr for four years.

Destroying multi-resistant pathogens

New nanomaterials such as fluorescing calcium phosphate nanoparticles were developed in a joint project of Matthias Epple and Jens Voskuhl. The surface of silica-coated calcium phosphate nanoparticles was covalently functionalized by azide groups. Alkynylated molecules can be covalently attached by copper-catalyzed azide-alkyne cycloaddition (CuAAC) and by strain-promoted azide-alkyne cycloaddition (SPAAC) via click chemistry, leading to a high packing density at the particle surface compared to the previous biotin-avidin binding concept. This was demonstrated for a number of dyes, e.g., FAM, TAMRA, Cy5, Alexa FluorTM 488. These nanoparticles (200 nm) are suitable for cellular uptake, as demonstrated by fluorescence imaging microscopy, confocal laser scanning microscopy, and structured illuminated microscopy. Correspondingly, other molecules can be bound by clicking, e. g., for targeting or as therapeutic agent. Overall, this paves the way for multimodal theranostic nanoparticles.[1]

Nanohybrids in theranostics

Michael Farle, Ulf Wiedwald, and co-workers, in collaboration with Russian colleagues, have developed magnetite-gold nanohybrids as an ideal all-in-one platform for theranostics. The octahedral 25 nm Fe_3O_4-Au hybrid nanoparticles exhibit bulk-like magnetic properties. Due to their high magnetization and octahedral shape, the hybrids show superior in vitro and in vivo T_2 contrast for magnetic resonance imaging (MRI) as compared to other hybrids and commercial contrast agents. The nanohybrids provide two functional surfaces for loading with fluorescent dyes and drugs which allow the simultaneous tracking of the nanoparticle vehicle and the drug cargo in vitro and in vivo. The delivery to tumors and payload release is demonstrated in real time by intravital microscopy.[2] Additionally, investigations on size-selected Fe_3O_4–Au hybrid nanoparticles of 6–44 nm (Fe_3O_4) and 3–11 nm (Au) size for improved magnetism-based theranostics were carried out. The 25 nm Fe_3O_4–Au nanohybrid exhibited the best characteristics for application as a contrast agent in MRI and for local heating using magnetic particle hyperthermia in aqueous and agarose systems. These nanohybrids used in vitro hyperthermia test for the 4T1 mouse breast cancer cell line demonstrated efficient cell death and nanoparticle visualization.[3]

Non-invasive, target-based cancer treatment

Daniel Erni and his work group studied the effect of hepatic vein on gold nanoparticle-mediated hyperthermia in liver cancer. The gold nanoparticle-mediated hyperthermia is a non-invasive, target-based cancer treatment with significantly reduced side effects compared to conventional treatments. A multiphysics simulation model was performed to investigate the case of a liver tumor located in the vicinity of a hepatic vein. Then, size-optimized gold nanorods are embedded in the liver, and the temperature raise under CW laser illumination is calculated, while taking into account the convective heat transfer through blood perfusion. The results show that an effective temperature raise is barely achievable when the tumor is located in the vicinity of the hepatic vein due to the heat drain into the blood stream. Moreover, it has been proven that for up to 90% of vein occlusions the temperature raise is not effective for tumor ablation.[4]

In a collaborative effort of Daniel Erni and Sebastian Schlücker‘s groups, computational studies and optical single-particle experiments were performed in order to evaluate the signal brightness of molecularly functionalized plasmonic nanoparticles for diagnostic purposes. Specifically, different classes of plasmonic nanoparticles such as gold nanoparticles,

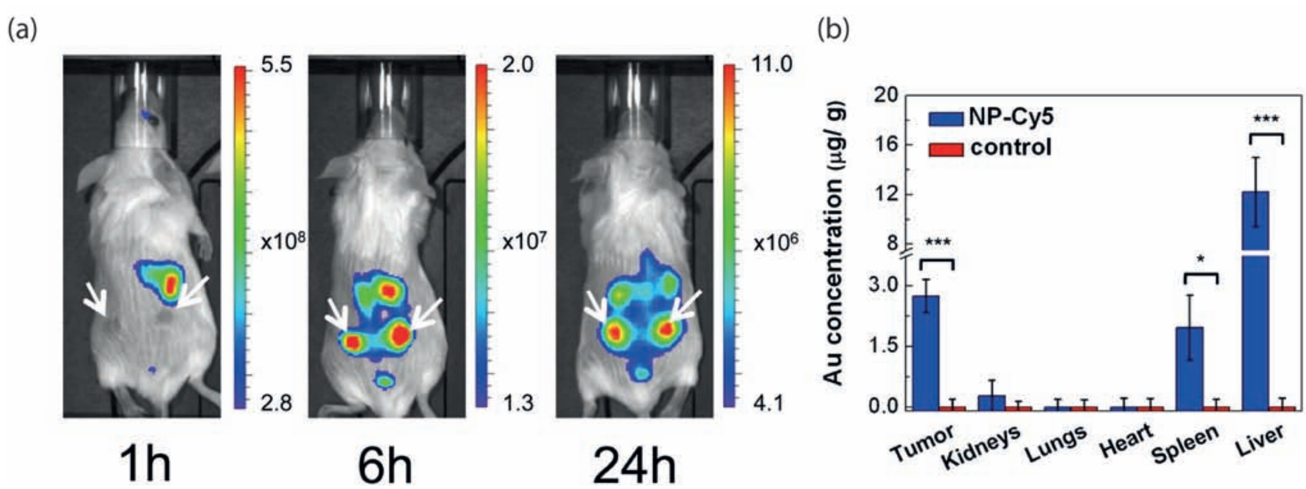

Fig. 1: (a) Photos of mice: NP-Cy5 accumulation in 4T1 tumors.
(b) Biodistribution of NP-Cy5 in 4T1 tumor-bearing mice 24 h after injection (6.6 mg·kg–1 Fe3O4, 1.0 mg·kg–1 Au). (Farle group)

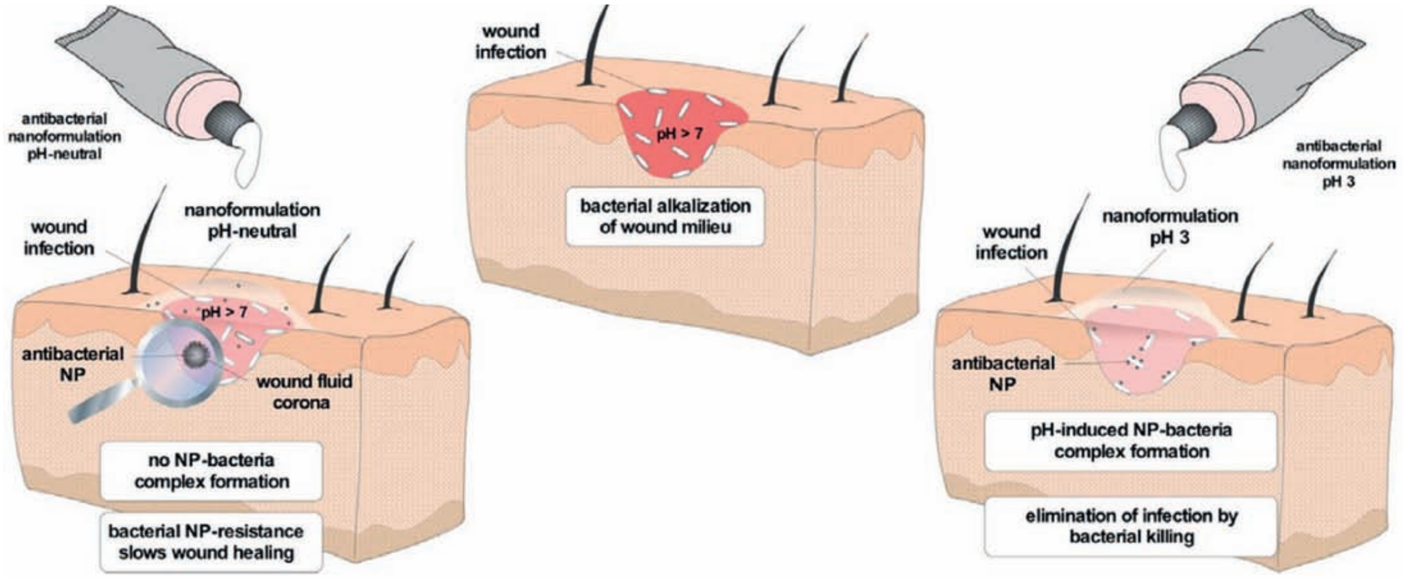

Fig. 2: Scheme of how low-pH nanoantibiotic formulation may improve therapy of skin infections in humans. (Knauer group)

hollow gold/silver nanoshells, gold nanostars, and gold core/gold satellite particles were tested for their signal brightness in surface-enhanced Raman spectroscopy (SERS) as an ultrasensitive detection technique in nanodiagnostics. Correlative SERS/SEM experiments have enabled the identification of single particles by electron microscopy as well as the characterization of both their elastic (LSPR) and inelastic (SERS) scattering spectra. Experimental observations were compared with predictions from FEM computer simulations. For single nanostars and core/satellite particles detectable SERS signals are shown.[5] The very bright core/satellite particles were then integrated in lateral flow assays (LFA) with clinical serum samples. A 15-fold improved sensitivity in comparison to commonly used assays and a fast readout (5 sec) via an in-house developed portable SERS reader with line illumination for point-of-care testing (POCT) could be achieved.[6]

Self-evolving structures

Based on a new model of the possible origin of life, Christian Mayer and co-workers proposed an efficient and stable system undergoing structural reproduction, self-optimization, and molecular evolution. The proposed system could also become a model for the formation of self-evolving structures, leading up to the creation of the first living cell. The system is formed by the interaction of two cyclic processes: one offers vesicles as the structural environment, the other supplies peptides from a variety of amino acids as versatile building blocks. Structures growing in a combination of these two cycles can support their own existence, to undergo chemical and structural evolution, and to develop as yet unpredicted functional properties. The key mechanism is the mutual stabilization of the peptides by the vesicles and of the vesicles by the peptides together with a constant production and selection of both. Clear evidence for a vesicle-induced accumulation of membrane-interacting peptide could be identified by LC-MS. The studied peptide has an effect on the vesicles, leading to (i) reduced vesicle size; (ii) increased vesicle membrane permeability; and (iii) improved thermal vesicle stability.[7]

Model for the formation of self-evolving structures

Mayer and Epple, along with co-workers, coated ultra-small gold nanoparticles (1.8 nm) with L-cysteine. By employing isotope-labeled cysteine, the surface structure and the coordination environment of the cysteine ligands on the nanoparticle were studied using ^{13}C- and ^{15}N-NMR spectroscopy. This was necessary for the interpretation of the complex 1H-NMR spectra, which could otherwise not be unambiguously assigned. By using the DOSY technique it was shown that the organic ligand is only present at the gold nanoparticle surface, with no residual cysteine molecules in the solution. The particle size data and the NMR-spectroscopic analysis showed three different binding sites for cysteine in the gold nanoparticle surface and a particle composition of about Au174(cysteine). This can be used to identify possible binding sites for cysteine with a different crystallographic environment.[8]

Serious respiratory tract diseases can be caused by airborne fungal pathogens (e.g., aspergillus fumigatus). Shirley Knauer and associates have demonstrated, that by using controlled nanoparticle models, those nanoparticles without specific functionalization rapidly and stably assemble on fungal spores. The complex formation of nanoparticle spores was enhanced by small nanoparticle size and was reduced in a concentration dependent manner by the formation of environmental or physiological biomolecule coronas. The assembly of nanoparticle spores affected their pathobiology and reduced the sensitivity against defensins, uptake into phagocytes, lung cell toxicity, and TLR/cytokine-mediated inflammatory responses. Nanoparticle-spore complexes were detectable in the lung tissue of mice after infection and were less efficiently eliminated by the pulmonary immune defense. This has resulted in enhanced A. fumigatus infections among immunocompromised animals. Collectively, the assembly of nanoparticle-fungal complexes affects their (patho)biological identity and may cause impacts on both environmental and human health.[9]

Nanoantibiotics

Furthermore, Shirley Knauer‘s group identified the first resistance mechanism specific for nanoantibiotics and provided a novel explanation as to why nanoantibiotics show reduced activity in clinically relevant environments. Nanoparticles are being investigated as novel antibiotics but are often inefficient in practical applications. It has furthermore been demonstrated that the resistance to antibiotics, mediated by biomolecule coronas acquired in pathophysiological environments, especially the antibiotic activity of metal nanoparticles against multidrug-resistant clinical isolates (MDR) strongly depends on a physical binding to pathogens. The nanoparticle-bacteria complex formation was enhanced due to the smallness of the particle. However, complex formation and MDR killing effects could be restored by low-pH nanoparticle formulations, thereby breaking bacterial resistance. Two independent in vivo models, *Galleria mellonella* and mice, show that low pH-induced complex formation was essential in order to significantly inhibit MDR *Staphylococcus aureus* skin wound infections with silver nanoparticles. The Knauer group recommends their model for studying the therapeutic and/or toxicological impact of nanoformulations in vivo prior to performing extensive studies in mammals.[10]

Artificial blood in a physiological environment

In the group of our new CENIDE member Katja Ferenz from the University Hospital Essen (UKE), an investigation on albumin-derived perfluorocarbon-based capsules (A-AOCs) as artificial oxygen carriers by means of holographic optical trapping was performed in cooperation with Cemal Esen‘s group (Applied Laser Technologies, Ruhr-University Bochum). The aim of this study is the characterization and provision of the holographic optical tweezer (HOT) to investigate individual A-AOCs for future use as artificial blood in a physiological environment. Furthermore, the motion behavior of capsules in a ring-shaped or vortex beam is being analyzed. HOT was successfully applied for initial examinations of surface interactions between A-AOCs in an experimental in vitro setting, and was highly effective in mimicking the (in vivo) physiological conditions of blood plasma.[11]

In addition to the selected highlights from our CENIDE research activities, it is worth mentioning that NanoBio materials benefits from the full spectrum of advanced instrumental analytics (AUZ, DLS, NTA, ADC, AFFF) combined with scalable colloid synthesis from liter scale-batch.

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NANOMATERIALS IN ENERGY TECHNOLOGY

The sustainable generation of usable energy and its storage in particular are among the major challenges of the 21st century – something we are working on.

In NanoEnergy Technology, CENIDE has been tackling the question of how nanomaterials can be used profitably for energy technology, especially in the field of energy conversion and energy storage. For this purpose, the state-of-the-art NanoEnergieTechnikZentrum (NETZ) research building has been established to ensure the continued success of this fundamental work.

Within CENIDE's NanoEnergy focus, various approaches of nanoscale materials related to batteries, fuel cells, photovoltaics, thermoelectrics, and light emitters are addressed from a theoretical, synthesis and processing point of view. The activities in the field of catalysis expanded significantly and now form an independent focus area within CENIDE .

Fuel cells

In proton exchange membrane fuel cells (PEMFCs), the activity and stability of catalysts (usually platinum nanoparticles on carbon) remains low due to kinetic limitations and carbon corrosion/platinum loss leading to high costs and limited lifetimes of the fuel cell. Within the cooperation between Sven Reichenberger's and Stephan Barcikowski's group and The Hydrogen and Fuel Cell Center ZBT, laser-ablation in the liquid phase has been employed to generate high-purity nanoparticles, enabling a direct contact to the carbon support and hence very good conductivity. Using these particles, a PEM fuel-cell demonstrator was built and tested under realistic conditions. Improved catalyst stability and activity was found in comparison to a commercially available reference catalyst.[1]

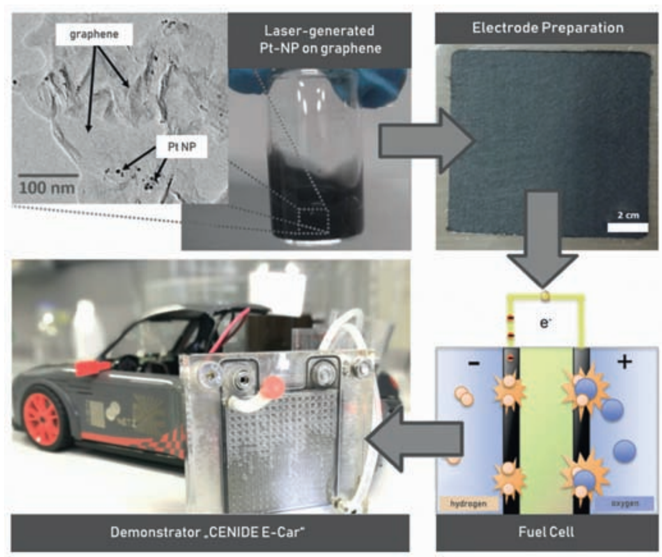

Fig. 1: Graphene-supported platinum particles and their demonstration in fuel cells.

High-performance batteries

Electrically contacting active materials is also crucial for high-performance battery storage materials. Gas-phase synthesized graphene was successfully used by Hartmut Wiggers's group to further enhance the already excellent performance of gas-phase synthesized silicon nanoparticles towards nanocomposites for Li-ion battery anodes. Electrochemical testing revealed that the gas-phase graphene significantly improves the long-term stability and Coulombic efficiency of the composite compared to pristine silicon.[2]

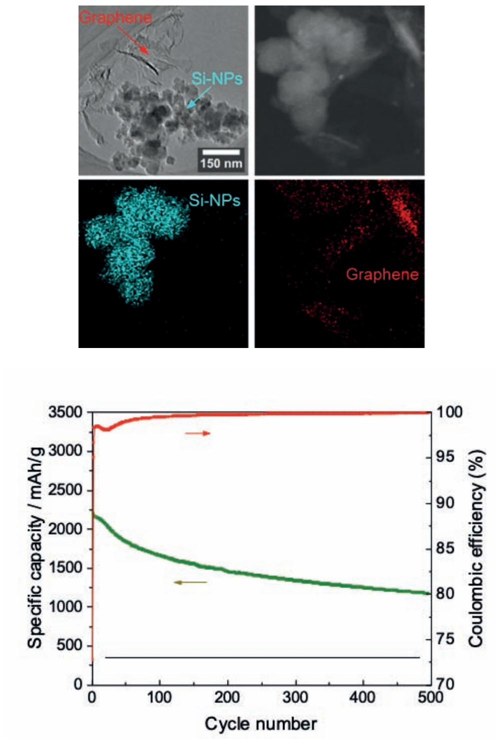

Fig. 2: Morphological and elemental structure of silicon/graphene nanocomposites and their outstanding electrochemical performance (black line: conventional graphite for comparison).

When designing nano-Si electrodes for lithium-ion batteries, the detrimental effect of the c-$Li_{15}Si_4$ phase formed upon full lithiation is often a concern. In a collaboration with Argonne National Labs, Hartmut Wiggers's team investigated the properties of gas-phase synthesized Si nanoparticles concerning parasitic reactions of the metastable c-$Li_{15}Si_4$ phase with the non-aqueous electrolyte. The use of small Si nanoparticles (~60 nm) and the addition of fluoroethylene carbonate additives played such a decisive role in the parasitic reactions that the c-$Li_{15}Si_4$ phase could disappear at the end of lithiation. This suppression of c-$Li_{15}Si_4$ improved the cycle life of the electrodes with little loss of specific capacity.[3]

In the case of batteries, but also in the case of other emerging fields like fuel-cell membranes, nanoparticles are key for sustainable technologies. But there are hardly any processes suitable for large-scale, industrial-style production. This is what the newly appointed Junior Professor Doris Segets wants to change, but first of all, she wants to clarify the basics: to do this she will analyze the properties of the particles, for example to understand how they behave in contact with certain liquids. If it is possible to distribute the particles evenly, this results in an ink from which will alow structured, functional layers to be printed for numerous applications. Particular important for this task are various coating facilities, including roll-to-roll coating for large-scale electrodes, in the "Linked Facility" in NETZ.

Thermoelectricity …

… plays an important role in energy conversion and recuperation of waste heat. Rossitza Pentcheva's group is exploring novel mechanisms for improving thermoelectrics from transition metal oxides and their heterostructures from first principles by high-performance computer simulations. The group demonstrated that the confinement-and strain-driven metal-to-insulator transition in $(LaNiO_3)_1/(LaAlO_3)/_1(001)$ perovskite superlattices leads to a strongly enhanced thermoelectric response comparable to some of the best-performing oxide systems. Epitaxial strain emerges as a control parameter in place of the conventional impurity doping. This finding established oxide systems at the verge of a metal-to-insulator transition as promising candidates for thermoelectric applications.[4]

Accurate determination and comprehensive understanding of the intrinsic c-axis thermal conductivity κ_c of thermoelectric layered Sb_2Te_3 is essential for optimizing the figure of merit in thin-film devices via heterostructures and defect engineering. Stephan Schulz's group determined κ_c of PVD-grown epitaxial Sb_2Te_3 thin films on Al_2O_3 substrates. At room temperature, they obtain κ_c= 1.9 W/mK, which is much smaller than the in-plane thermal conductivity and even the thermal conductivity of nanocrystalline films.[5]

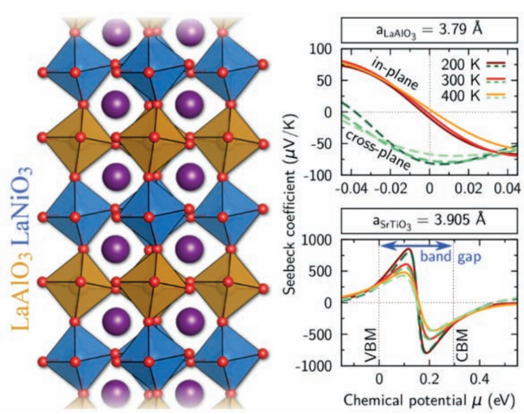

Fig. 3: Optimized crystal structure of a $(LaNiO_3)_1/(LaAlO_3)/_1(001)$ superlattice and its thermoelectric performance for two different substrates.

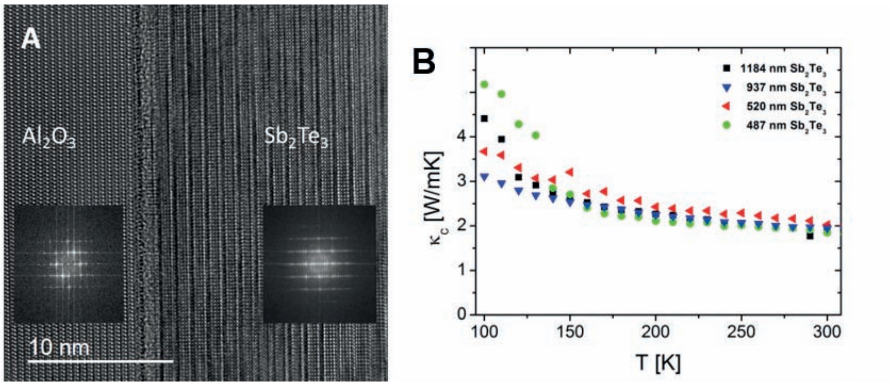

Fig. 4: (A) HRTEM image and FFTs of an Al_2O_3–Sb_2Te^3 interface (191 nm thick), demonstrating epitaxial c-axis oriented film; (B) C-axis thermal conductivity κ_c of the PVD grown Sb_2Te_3 films of different thicknesses after correction for Kapitza resistances and the contribution of the SiO_2 insulation layer.

So far, the use of thermoelectric generators in high-temperature applications is limited because the bonding contacts between the semiconductor and metal electrodes are not capable of withstanding thermal-mechanical stress and alloying of the metal-semiconductor interface. In collaboration with partners from Dresden, Roland Schmechel's and Hartmut Wiggers's groups demonstrated a new concept for high-temperature thermoelectric generators by replacing the metallization and electrode bonding on the hot side of the device by a p-n junction between the two semiconductor materials. They demonstrated a p-n junction device made from nanocrystalline silicon that is competitive in efficiency and power output to conventional devices of the same material, but with the important advantage of sustaining high hot-side temperatures and oxidative atmospheres.[6]

The theoretical assessment of materials for thermoelectrics is one of the topics that led theoretician Anna Grünebohm (former UDE, now at Ruhr-University Bochum) to winning an Emmy Noether Junior Research group. An important aim is to replace expensive and toxic materials, e.g, by oxides with a perovskite structure. Many of these materials can be permanently electrically polarized and have other properties that make them promising candidates for sustainable technologies: efficient cooling, the use of waste heat, or the short-term storage of electrical energy.

Solar cell technologies

Recent years have seen substantial efficiency improvements for a variety of solar cell technologies as well as the rise of a new class of photovoltaic absorber materials, e.g., metal-halide perovskites. Conversion efficiencies that aproach the thermodynamic limit require a physical description of the corresponding solar cells that is compatible with those limits. In a paper from Thomas Kirchartz's group, the recent work on the interdependence of basic material properties of semiconductor materials with their efficiency potential as photovoltaic absorbers is assessed. The connection of the classical Shockley–Queisser approach, with the band-gap energy as the only parameter, to a more general radiative limit and to situations where non-radiative recombination dominates is discussed. The authors delineate a consistent loss analysis that enables a quantitative comparison between different solar cell technologies. Bulk materials properties that influence the photovoltaic performance of a semiconductor such as absorption coefficient, density of states, or phonon energies are considered. It has been demonstrated that varying these properties strongly influences the optimized design of a solar cell but not necessarily its achievable efficiency.[7, 8]

Light concentration …

… opens up the path to enhanced material efficiency of solar cells via increased conversion efficiency and decreased material requirement. For true material saving, a fabrication method allowing local growth of high-quality absorber material is essential. Martina Schmid's group presents in cooperation with partners from BAM and IKZ (both in Berlin) two scalable femtosecond-laser-based approaches for bottom-up growth of $Cu(In,Ga)Se_2$ micro islands utilizing either site-controlled assembly of In(Ga) droplets on laser-patterned substrates during physical vapor deposition, or laser-induced forward transfer of (Cu,In,Ga) layers for local precursor arrangement. The $Cu(In,Ga)Se_2$ absorbers formed after selenization can

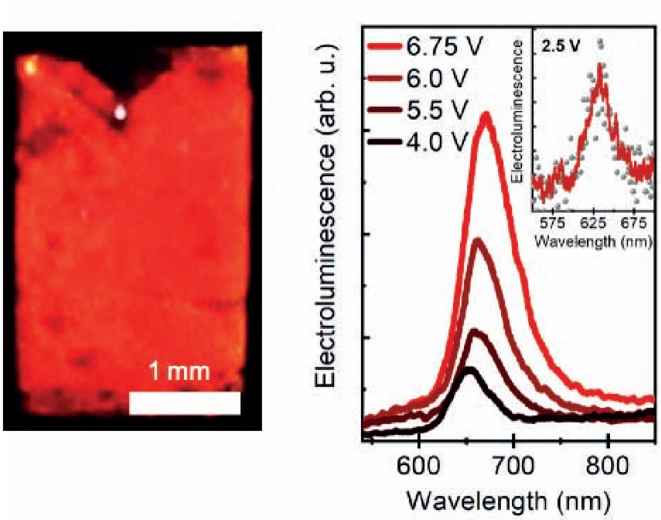

Fig. 5. Left: Large area electroluminescence from a p-n light emitting device containing a monolayer of WS_2 as active material. Right: Electroluminescence spectra of the device for different operation voltages demonstrating a turn-on voltage of 2.5 V.

deliver working solar devices showing efficiency enhancement under light concentration.[9]

Martina Schmid's group also numerically evaluated light-trapping based on dielectric nanoparticles in ultra-thin $CuIn_{1-x}Ga_xSe_2$ (CIGSe) solar cells. They found that for a significant light absorption enhancement, the preferred method is to integrate dielectric nanoparticles at the rear interface of the CIGSe/back contact and employ transparent conductive oxide back contacts. They demonstrated that under front illumination, low-index ($n = 1.5$), hemispherical nanoparticles cause significant light trapping. In contrast, under back illumination, the patterned ultrathin cells realize comparable absorption to the corresponding thick counterpart at a CIGSe thickness of only 300 nm. This suggests that patterned ultrathin CIGSe solar cells under back illumination are promising for both high efficiencies and reduced materials usage in industrial production.[10]

For large-area flexible lighting solutions, …

… light-emitting electrochemical cells (LECs) are promising because of their simple device architecture as well as the solution-based processing. The lack of deep-blue emitters, which are at the same time efficient, bright, and long-term stable, hampers the creation of white LECs. Ekaterina Nannen's group (former UDE, now at Hochschule Niederrhein) presented a hybrid device concept for the realization of white-light emission by combining blue colloidal quantum dots (QDs) and an Ir-based ionic transition-metal complex (iTMC) LEC in a new type of white QD-LEC hybrid device (QLEC). The QLEC devices show homogeneous white light emission with high color rendering index (up to 80), luminance levels above 850 cd/m^2, and a maximum external quantum efficiency greater than 0.2%.[11]

Fabrication of transition-metal dichalcogenides (TMDCs) like MoS_2 and WS_2 via metal-organic chemical vapor deposition (MOCVD) represents one of the most attractive routes to large-scale 2D materials layers. Although good homogeneity and electrical conductance have been reported recently, the relation between growth parameters and photoluminescence intensity – one of the most important parameters for optoelectronic applications – has not yet been discussed for MOCVD TMDCs. Gerd Bacher's group analyzed MoS_2 grown via MOCVD on sapphire (0001) substrates using molybdenum hexacarbonyl ($Mo(CO)_6$, MCO) and di-tert-butyl sulphide as precursor materials. A prebake step under H2 combined with a reduced MCO precursor flow increases the crystal grain size by one order of magnitude and strongly enhances photoluminescence with a clear correlation to the grain size[12]. In an important step towards device development, the scientists integrated WS_2 into a p-i-n layout for light emitters[13] and expanded this concept to a scalable approach using MOCVD grown WS_2 monolayers.[14]

Photonic liquids and crystals

In collaboration with scientists from Cambridge (UK), Aalto University (Finland), Pau (France) and St. Petersburg (Russia), André Gröschel's group has investigated the independent formation of photonic liquids and crystals of block copolymer micelles.[15] In nature there are colors everywhere. Animals and plants produce these not only by pigmentation, but also by structural coloring. Examples are colorful iridescent opals or the blue morpho butterfly. These colors are produced by reflection and interference of the light rays on periodic microstructures and can persist for centuries. The Emmy Noether Junior Research Group Leader Gröschel and his team show for the first time the process for the hierarchical development of photonic structures starting from polymer chains of a few nanometers in size, through spherical block copolymer micelles to photonic lattices. This makes it possible for the first time, with the exception of large core-shell virus particles, to produce photonic crystals from self-assembled nanoparticles.

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„CONTENT OUGHT TO BE SET, BUT PEOPLE SHOULDN'T."

Since December 2018, engineer Prof. Dr.-Ing. Doris Segets has been conducting research in the field of 'Process Engineering of Electrochemical Functional Materials' at the NanoEnergieTechnikZentrum (NETZ). An interview about team spirit, scientific toolboxes and people.

NETZ at a glance

- Pilot-scale plants for the synthesis of nanomaterials from the gas phase with adjacent linked facilities
- State-of-the-art microscopy center
- Linked facilities for a pilot-scale synthesis and processing chain
- Photovoltaic system and weathering test surface for functional coatings of all kinds
- Highly effective heat exchangers for heating and cooling the building with waste heat from large appliances

You were appointed to the UDE in December 2018 and have been working at NETZ since then. How did it appear to you before, as an outsider?

If you look at a German university map on the subject of „nano", CENIDE is the location. So I arrived at Duisburg Central Station for my interview on a rainy April day. To be honest, I actually wanted to turn around again. But when I was at the NETZ, the sun appeared behind the clouds – actually and figuratively: I immediately felt this interdisciplinary spirit between the working groups, this vivid cooperation gave me a good feeling right from the start. Nanotechnology, especially NanoEnergy, simply requires the cooperation of many disciplines. Engineers for technology, chemists and physicists for the basics, the role of the material sciences are self-evident. In the NETZ, we do have this large pool of different experts. And in the background, there's excellent science management only for nanotechnology, which holds the scientists' back for their actual task – research.

Application-oriented research at the NETZ currently concentrates on thermoelectrics, catalysis, photovoltaics, fuel cells and battery technology in order to find solutions for important issues in energy technology. Where do you currently see the greatest potential?

In photovoltaics, catalysis and battery technology. In the light of the 'Energiewende' in Germany, these disciplines form the crucial toolbox.

Previously, you worked in Erlangen, a region that differs greatly from the Ruhr region. With this in mind, how do you assess the geographical proximity to many partners at this specific location?

I particularly see the affiliated institutes as an opportunity that cannot be overestimated. I already work closely with the Zentrum für BrennstoffzellenTechnik (ZBT) right next door, and the same applies to two other affiliated institutes. This is a decisive locational advantage that helps to shape the transition from an academic lighthouse to a marketable technology. The second advantage of the Ruhr Area is its human resource. The region has already learned to welcome foreigners with open arms – whether it is a Franconian or an Indian (laughs). This results in a good international mix of people and skills, which is particularly important in an academic context.

Prof. Dr.-Ing. Doris Segets, Process Technology for Electrochemical Functional Materials.

If you look at your research in the NETZ context – what are your plans for the beginning?

I see myself as an interface between synthesis and application. Therefore, I have two things in mind for the near future: On the one hand, I want to get material from as many synthesis groups as possible to test, in order to know what I am dealing with. On the other hand, I receive slurries or inks for characterization and coating from the application side. This allows me to check the application range, to explore my own limits and to find out exactly what is needed to make a good ink and how to process it further into high performance electrodes and devices. That way I want to bridge the gap between synthesis and application, academia and industry and the various disciplines involved.

Along with your appointment, you have taken responsibility for the modular coating system in the linked facilities. So, what concrete plans do you have for this in the near future?

Together with a postdoc, who has been with us since June, we are currently putting the plant back into operation. We are defining two to three model cases that we will start with: We are working with a layer of battery material made of graphene-coated silicon and in parallel with material for fuel cells. In this way, we can determine where we stand: What can the plant do actually? Where are the white spots? On that basis, we want to develop a characterization cascade with the aim of quickly separating good from bad results and to establish process-structure-property relationships. We want to implement this online in the plant, digitalize, as soon as possible. By doing so we will be able to assess directly what we need and to identify optimum formulation and coating processes for high performance materials.

With Prof. Corina Andronescu and Prof. Malte Behrens, two working groups from catalysis are about to move into the NETZ. Have you already exchanged ideas, maybe already cooperation plans?

In terms of characterisation, functionalisation and structuring, we can immediately find docking points once every-one has settled in. Both will be central partners of my own research.

In contrast to other buildings at a university, NETZ has a board of directors, of which you are a member. Among other things, you decide on the allocation of laboratory and office space to working groups. Why is that necessary?

The building has a mission and a clear national assignment, which is partly due to the use of taxpayers‘ money. We must therefore carry out transparent checks and ensure that the most suitable working groups, who are visible and cooperative in the community, are allowed to conduct research in their field of NanoEnergy. Annual status meetings monitor this. After all, quality assurance – where all this is about – is achieved by setting functions and content but never people.

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FINDING THE NEEDLE IN THE HAYSTACK

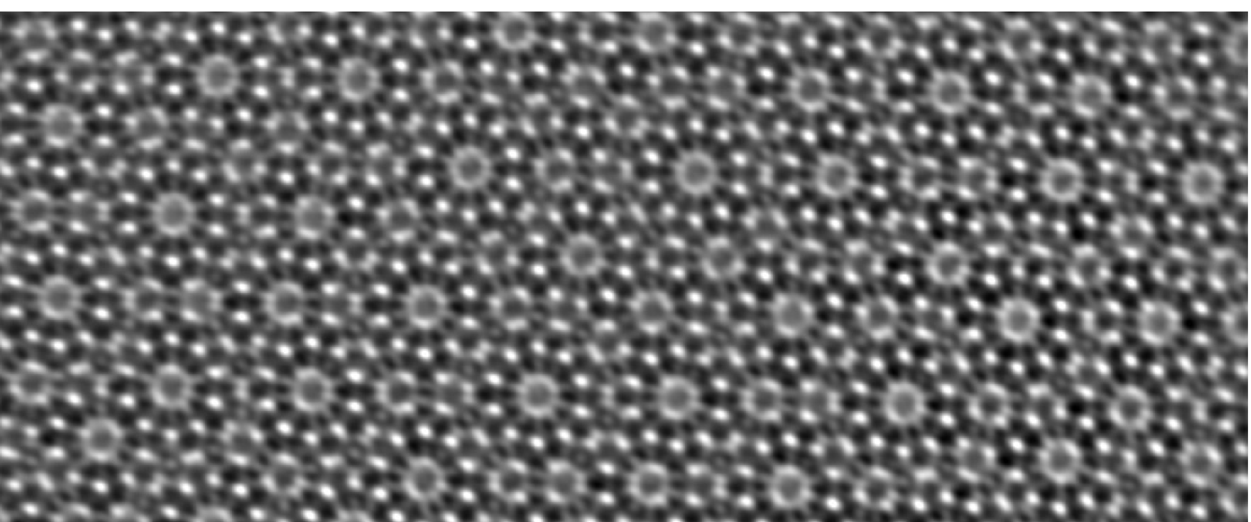
Is there a single iron atom hidden in 1,000,000 carbon atoms? Are two elements linked by single or double bonds? The Interdisciplinary Center for Analytics on the Nanoscale (ICAN) has the answers.

The DFG Core Facility ICAN combines equipment, methods and technical competence for analytics on the nanometer scale. Complex analytical methods are required to optimize the processing and structure of new materials and to understand the underlying mechanisms. Investigations of this kind require a combination of expertise and experimental equipment that can rarely be found in a single location.

ICAN gives the university's research groups and cooperation partners the opportunity to have their samples analyzed by the most suitable methods: The characterization includes both static snapshots of the material structure as well as time-resolved processes that are important for the synthesis and functionality of the materials. As far as possible, the analyses take place under real technical conditions, including in-situ and ex-situ methods and even cover investigations on model systems.

The highly complex nature of the equipment requires special know-how for planning and carrying out the measurements. Given appropriate professional suitability and instruction, the instruments are personally accessible for users. Otherwise, ICAN advises on the selection of the methodology, carries out the measurements and – if desired – helps to interpret the results.

The Microscopy Center located in the NanoEnergieTechnikZentrum (NETZ) is a central location. Here, right next to the synthesis laboratories, special – mechanically damped and electromagnetically shielded – laboratories have been set up in which state-of-the-art equipment is operated in order to enable sensitive measurements with the highest resolution up to the atomic level.



HAADF STEM image of an AlCoNi quasicrystal. The white dots are CO and Ni atoms, which are seen from above.

ICAN
INTERDISCIPLINARY CENTER FOR ANALYTICS ON THE NANOSCALE

Large Equipment

- **Cs-corrected Transmission Electron Microscope (TEM):** Provides information about morphology, crystal structure, atomic defects, chemical composition and electronic structure on the sub-nanometer scale.
- **Time-of-Flight Secondary Ion Mass Spectrometer (TOF-SIMS):** Provides Information about chemical composition and structure of micrometer-sized areas with an information depth even below one nanometer.
- **Microfocus X-ray Photoelectron Spectrometer (XPS):** Provides information about chemical composition (quantitative), chemical structure and binding states in micrometer-sized areas with an information depth of a few nanometers.
- **Atomic Force / Scanning Probe Microscope (AFM/SPM):** Provides information about topography, size and heights of nanoobjects, mechanical, chemical and electronical/electrical properties on the nanometer scale.
- **Scanning Auger Electron Microscope (SAM):** Provides information about chemical composition, in some cases also chemical structure and binding states on the nanometer scale.

Who can benefit from ICAN?
Dr. Ulrich Hagemann, physicist and ICAN scientist, is responsible for XPS and SAM: “ICAN is accessible to UDE researchers, cooperation partners from science and industry, but also to industrial customers in general and even private persons. In the end, the samples and the scientific questions are the decisive factors, not the customer: The task must match our equipment.”

The Director’s Perspective

Prof. Meyer zu Heringdorf, in your opinion as ICAN’s Scientific Director, what makes it unique?
MzH: ICAN offers modern and highly sophisticated methodology for surface analysis. The five large-scale analytical instruments of ICAN are complemented by many analysis and sample-preparation tools. What makes ICAN special is the permanent scientific staff that operates and maintains the instruments, but also offers training and advice. If users tell ICAN‘s scientists what information they need (and maybe why they need it), the staff will assist them in developing a strategy to obtain the results.

The User’s Perspective

An interview with PhD student and ICAN user Sebastian Tigges.
Mr. Tigges, what do you particularly appreciate about ICAN as a user?
ST: That’s definitively the proximity to our own labs and the combination of instruments. It makes it easy to validate yourself again and again, to check your own theories straightforwardly on different devices. I also like the openness of the ICAN staff: they help with comprehension problems with literature and evaluate the data on request: What do they say, where is the limit? Since ICAN does not have its own agenda, I get neutral advice on my projects.

What experience have you had with consulting?
ST: I was already familiar with the methods in general, but still wanted to check them out. Dr. Heidelmann recommended tomography as an alternative method at the TEM, and he was right: The result has helped me on a lot. (Laughs) I can handle the TEM myself, but when Markus operates it, it looks like playing the piano.

Nevertheless, as a regular user, you also operate the devices yourself. What advantage do you think it has?
ST: Like everyone else, I plan my measurements via online equipment calendar. As an independent user, however, I can take the time I need and measure without any hurry.

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„GET OUT OF YOUR OWN BOX!“

They are the elected speakers of YOURNET: Dr. Anna Mechler from the Max Planck Institute for Chemical Energy Conversion in Mülheim and Dr. Miriana Vadalà from the Institute of Materials Science at the UDE. An interview with the scientists about the important exchange at eye level.

YOURNET
YOUNG
RESEARCHER
NETWORK

Becoming a YOURNET member

You are a junior professor, research assistant or postdoc in nanosciences and you fancy a career in research?

Just write a formless e-mail to introduce yourself and join one of YOURNET's meetings to get to know the others. Of course the membership is free of charge.

Would you briefly introduce YOURNET to us?

MV: It's a great network for young scientists from the nanosciences to exchange ideas and get connected with colleagues at eye level. Scientifically, of course, but also privately. And there is information and events on different career paths.

Dr. Mechler, you are not working at the UDE, but you are part of YOURNET. So, who can become a member? Are there any criteria?

AM: First of all, there is the career level you are at. YOURNET is interesting if you are a group leader or postdoc. In addition, of course, there is the focus on nanosciences, which should play a central role in one's own research. Scientists from the UDE, but also from the affiliated and cooperating institutes are very welcome, as you can see from me. As I see it, it's great to get out of my own box and experience research at university.

Why is it important for young scientists to network separately for themselves?

MV: When you are with people on the same career level, there are fewer inhibitions to discuss things or problems you encounter. We often notice that many people are dealing with the same topics. That gives us the chance to exchange experiences and helpful tips. And you might not always want to go to the professor, even if they have time. In YOURNET there is a relaxed atmosphere and it's easy to deal with.

What do you see as YOURNET's greatest strength? What makes the network particularly attractive for members?

AM: To me, this is definitely the exchange among each other. Discussions such as What do I do? Where do I want to go? How do I do that? It's also often about soft skills or everyday challenges that simply

belong to our work. For example, how to supervise PhD students. In addition, we have workshops, lectures, joint ventures. It's a well-rounded thing.
MV: I very much like the fact that we are so different. We have different opinions and approaches. I find it particularly exciting that some of us have already worked in industry and bring this perspective to our more academic circle.

Do you have a specific example of an interdisciplinary exchange or a jointly launched project?
AM: As standard, we help each other with equipment: For example, PhD students of mine recently needed a Zeta potential measuring device, another group had one. So we were able to measure uncomplicatedly and free of charge.
MV: Of course we hope that something like this will evolve and that we will be able to start joint projects, but this takes time.

Are there other networks of young scientists at the UDE or within the UA Ruhr? If so, are there any thoughts of exchanging ideas?
AM: Yes, there are. At the Materials Chain workshop in autumn we will present YOURNET and hope for two things: new members from the UDE, but also the exchange with these other networks from the nano and materials sciences in Bochum and Dortmund.

What joint training courses are you currently planning?
MV: We have already had training in funding and leadership, this year similar workshops are on the agenda.

YOURNET is a scientific network. Why do you nevertheless emphasize the private level on your website, for example with joint leisure activities?
AM: We are all more than just scientists. Because we are about the same age, we also have private overlaps, similar lifestyles. For example, ‚How do I balance children and work?' is a topic that is a big issue for many people.

What is the advantage of a dual leadership and how do you two complement each other?
MV: If there is something that needs to be clarified in the short term, we can coordinate, and share the responsibility.
AM: And it's an honorary position, so we can simply share the work. In addition, we come from different institutes, different disciplines and therefore do not necessarily always represent the same interests. That's what makes it so interesting.

What goals have you both set yourself for YOURNET?
AM: We want to grow, attract more members.
MV: Right. And now that YOURNET is established, we want it to become more visible. It would be great if we could initiate the first joint projects beyond the boundaries of working groups or institutes.


Always looking forward to new arrivals: Dr. Miriana Vadalà (left) and Dr. Anna Mechler (right) .

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DFG-funded Collaborative Research Centers/Transregios (CRC/TRR)

CRC 1242: Non-Equilibrium Dynamics of Condensed Matter in the Time Domain (since 2016)
CENIDE Main Research Area:
Dynamic processes in solids
Contact: Prof. Dr. Uwe Bovensiepen
(Spokesperson)

CRC 1093: Supramolecular Chemistry on Proteins (since 2014)
CENIDE Main Research Area:
NanoBio materials
Contact: Prof. Dr. Thomas Schrader
(Spokesperson)

CRC/TRR 247: Heterogeneous Oxidation Catalysis in the Liquid Phase – Mechanisms and Materials in Thermal, Electro-, and Photocatalysis (since 2018)
CENIDE Main Research Area: Catalysis
Contact: Prof. Dr. Malte Behrens
(Spokesperson)

DFG-funded Coordinated Priority Programs (SPP)

SPP 2122: Materials for Laser-based Additive Manufacturing (since 2018)
Contact: Prof. Dr. Stephan Barcikowski
(Coordinator)

SPP 1980: Sprayflame Synthesis (since 2017)
CENIDE Main Research Area:
Gas-phase synthesis
Contact: Prof. Dr. Christof Schulz
(Coordinator)

DFG-funded Participation in Priority Programs (SPP)

SPP 1708: Material Synthesis near Room Temperature (since 2014)
CENIDE Main Research Area:
NanoEnergy technology
Contact: Prof. Dr. Stephan Schulz
(Project member)

SPP 1681: Field Controlled Particle Matrix Interaction: Synthesis, Multi-Scale Modelling and Application of Magnetic Hybrid-Materials (since 2013)
CENIDE Main Research Area: Magnetism
Contact: Prof. Dr. Heiko Wende
(Project member)

SPP 1666: Topological Insulators (since 2013)
Contact: Prof. Dr. Stephan Schulz
(Project member)

SPP 1613: Fuels Produced Regeneratively Through Light-Driven Water Splitting: Clarification of the Elemental Processes Involved and Prospects for Implementation in Technological Concepts (since 2012)
CENIDE Main Research Area:
NanoEnergy technology
Contact: Prof. Dr. Rossitza Pentcheva
(Project member)
Prof. Dr. Malte Behrens
(Project member)
Prof. Dr. Markus Winterer
(Project member)

SPP 1599: Caloric Effects in Ferroic Materials: New Concepts for Cooling (since 2012)
CENIDE Main Research Area: Magnetism
Contact: Prof. Dr. Peter Entel
(Project member)
Prof. Dr. Michael Farle
(Project member)
Prof. Dr. rer. nat. Doru C. Lupascu
(Project member)
Prof. Dr. Heiko Wende
(Project member)
PD Dr. Markus Gruner
(Project member)

SPP 1538: Spin Caloric Transport (SpinCaT) (since 2011)
CENIDE Main Research Area: Magnetism
Contact: Prof. Dr. Peter Kratzer
(Project member)
Prof. Dr. Peter Entel
(Project member)
Prof. Dr. Michael Farle
(Project member)

SPP 1459: Graphene (since 2010)
CENIDE Main Research Area:
Dynamic processes in solids
Contact: Prof. Dr. Marika Schleberger
(Project member)
Dr.-Ing. Wolfgang Mertin
(Project member)

DFG-funded Coordinated Research Units (FOR)

FOR 2284: Model-based scalable gas-phase synthesis of complex nanoparticles (since 2015)
CENIDE Main Research Area:
Gas-phase synthesis
Contact: Prof. Dr. Christof Schulz
(Spokesperson)

Overview of current research projects

FOR 1993: Multi-functional conversion of chemical species and energy (since 2013)
Contact: Prof. Dr. Burak Atakan (Spokesperson)

DFG-funded Participation in Research Units (FOR)

FOR 1700: Metallic Nanowires on the Atomic Scale: Electronic and Vibrational Coupling in Real World Systems (since 2012)
Contact: Prof. Dr. Uwe Bovensiepen (Project member)
Prof. Dr. Michael Horn-von Hoegen (Project member)

FOR 1509: Ferroic Functional Materials – Multiscale Modelling and Experimental Characterization (since 2012)
CENIDE Main Research Area: Magnetism
Contact: Prof. Dr. Doru C. Lupascu
Prof. Dr. Heiko Wende (Project member)

DFG Core Facility

Interdisciplinary Center for Analytics on the Nanoscale (ICAN) (2017 – 2020)
Contact: Apl. Prof. Dr. Nils Hartmann (Project coordinator)

EU Projects

SAIL PRO – Safe and Amplified Industrial Laser PROcessing (2016 – 2019)
CENIDE Main Research Area: NanoEnergy technology
Contact: Prof. Dr. Stephan Barcikowski (Project manager)

NanoDome: Nanomaterials via Gas-Phase Synthesis: A Design-Oriented Modelling and Engineering Approach (2015 – 2018)
CENIDE Main Research Area: Gas-phase synthesis
Contact: Prof. Dr.-Ing. Andreas Kempf (Project member)
Prof. Dr. Christof Schulz (Project member)
PD Dr. Hartmut Wiggers (Project member)

NU-MATHIMO: New Materials for High Moment Poles and Shields (2013 – 2017)
CENIDE Main Research Area: Magnetism
Contact: Prof. Dr. Heiko Wende (Project member)

BMBF Projects

KontiKat – Kontaminationsfreie Herstellung und Aufbereitung lasergenerierter Nanopartikel in einer kontinuierlichen Prozesskette für die heterogene Katalyse (2017 – 2019)
CENIDE Main Research Area: Catalysis
Contact: Prof. Dr. Stephan Barcikowski (Project member)

NEMEZU – Neue edelmetalfreie Membran-Elektoden-Einheiten für Brennstoffzellen der Zukunft (2015 – 2018)
CENIDE Main Research Area: NanoEnergy technology
Contact: Prof. Dr. Stephan Barcikowski (Project member)
Prof. Dr. Angelika Heinze (Project member)

nanoGRAVUR – nanostructured materials – grouping for occupational health, consumer and environmental protection and risk mitigation (2015 – 2018)
Contact: Apl. Dr. Thomas Kuhlbusch (Project coordinator)
Dr. Tobias Teckentrup (Project management)

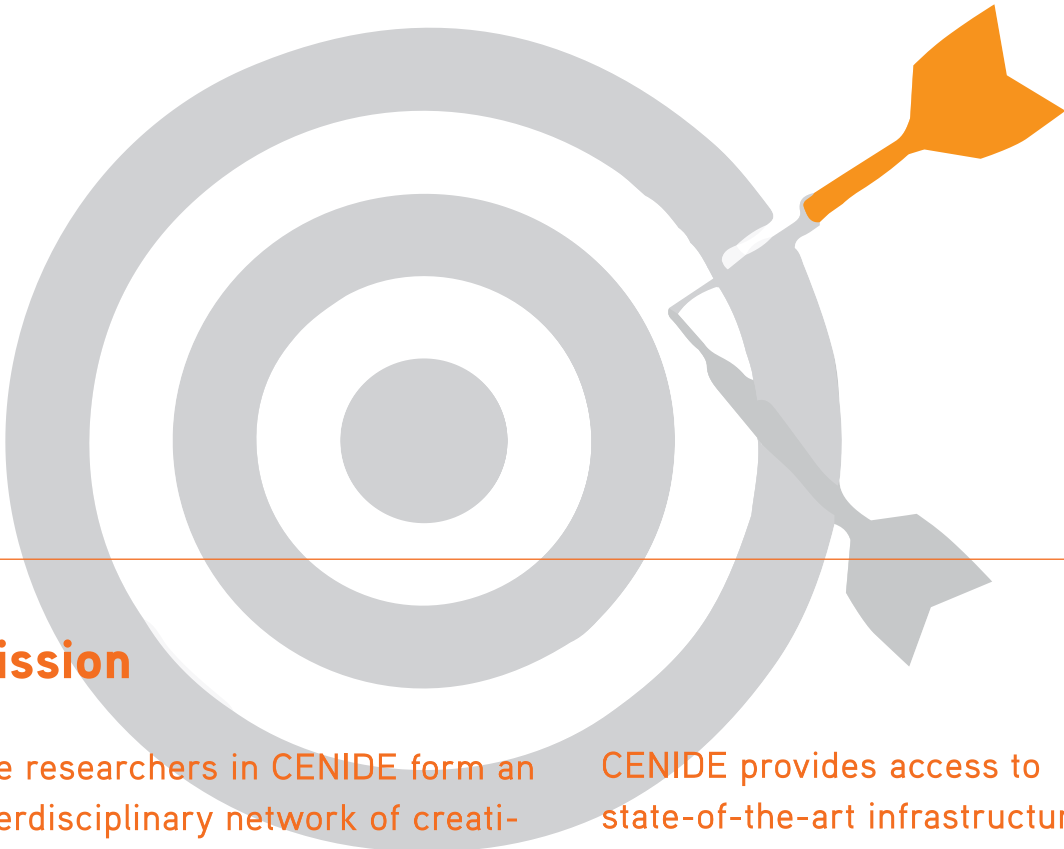
International Max Planck Research Schools (IMPRS)

IMPRS on Reactive Structure Analysis for Chemical Reactions (RECHARGE) (2015 – 2021)
CENIDE Main Research Area: NanoEnergy technology
Contact: Dr. Tobias Teckentrup (Project management)
Prof. Dr. Malte Behrens (Project member)
Prof. Dr. Christof Schulz (Project member)
Prof. Dr. Stefan Schulz (Project member)
PD Dr. Hartmut Wiggers (Project member)

IMPRS for Interface Controlled Materials for Energy Conversion (SURMAT) (2016 – 2021)
CENIDE Main Research Area: NanoEnergy technology
Contact: Dr. Tobias Teckentrup (Project management)
Jun.-Prof. Dr. Corina Andronescu
Prof. Dr. Gerd Bacher
Prof. Dr.-Ing. Stephan Barcikowski
Prof. Dr. Axel Lorke
Prof. Dr. Rossitza Pentcheva
Prof. Dr. Christof Schulz
Prof. Dr.-Ing. Doris Segets
Prof. Dr. Heiko Wende
PD Dr. Hartmut Wiggers
(Project members)

DAAD Projects

Partnership with Japan and Korea (PAJAKO) (2017 – 2020)
CENIDE Main Research Area: NanoEnergy technology
Contact: Dr. Tobias Teckentrup (Project management)



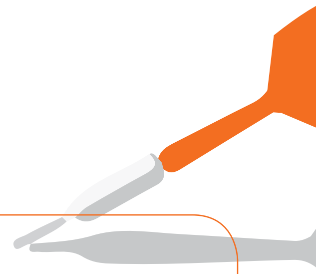
Mission

The researchers in CENIDE form an interdisciplinary network of creative minds that fosters collaboration across disciplines, bridging the gap between fundamental academic research and industrial implementation.

CENIDE coordinates and promotes the advancement of science in chemistry, physics, engineering, biology, and medicine with focus on:

- Catalysis
- Dynamic processes in solids
- Gas-phase synthesis of nanomaterials
- Magnetic materials
- Nanomaterials for health
- Nanotechnology in energy applications

CENIDE provides access to state-of-the-art infrastructure such as the unique research building NanoEnergieTechnikZentrum (NETZ) and the Interdisciplinary Center for Analytics on the Nanoscale (ICAN). CENIDE supports the creation and management of collaborative research activities for its members and partners from academia and industry. The stimulating research environment attracts high potentials and provides students and junior scientists with an ideal basis for further development.

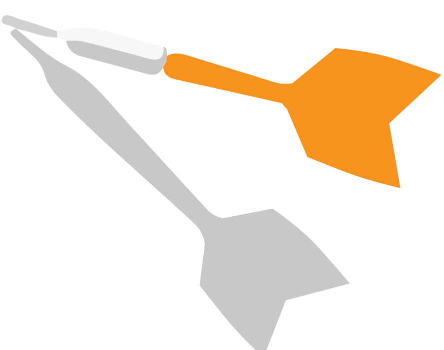


Objectives and tasks

- Coordination of nanoscience at the UDE in research and teaching
- Coordination of public image and enhancement of (international) visibility with regard to field-specific expertise and strengths
- Research and technology transfer in nanotechnology

Vision

The Center for Nanointegration Duisburg-Essen (CENIDE) is internationally recognized for its cutting-edge materials research and development: Integrating the fundamental understanding on the nanoscale to create new sustainable solutions for major societal challenges in the fields of energy, information technology, and health.



History

- Founded: June 2005
- Head office established: November 2006
- Research center (with bye-laws): Since May 2007

Location

In recent decades, the five-million metropolis of the Ruhr region has transformed itself from a mining and steel centre to a modern location for business and science.

But even the structurally transformed Ruhr region has not yet seen anything like the research building NanoEnergieTechnikZentrum, which costs around 46 million euros and covers 3,900 m^2 main useable area including 36 laboratories and 66 offices. Since the beginning of 2013, around 120 scientists and partners from industry have been working together on one goal.

Together they research and analyse new materials for energy applications and develop scalable processes for their manufacture and processing. The „linked facilities“ enable our chemists, engineers and physicists to work together in an uncomplicated and efficient way.

Services

For CENIDE members and associates

- Research management
- Analytics services (ICAN)
- Promotion young researchers (e.g. YOURNET)
- Press, public relations and marketing
- Event management
- Hub for information

For externals

- Analytics services (ICAN)
- Nano schools laboratory
- Degree course Nano Engineering

Collaboration and network

(Selection)

USA & Canada

- Stanford University (USA)
- University of Pennsylvania (USA)
- University of Minnesota (USA)
- University of California (USA)
- University of Waterloo (Canada)

Europa

- Cambridge University (UK)
- ETH Zurich (Swiss)
- Lund University (Sweden)

Asia

- University of Tsukuba (Japan)
- Huazhong University (China)
- Chinese Academy of Science (Beijing, China)
- National Tsing Hua University (Taiwan)

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Research Topic

Electrochemical Catalysis

- Synthesis and in-depth characterization of non-noble metal based electrocatalysts for energy conversion and synthesis of platform chemicals
- Electrochemical investigation of hybrid electrocatalysts for the oxygen evolution and oxygen reduction reactions, the hydrogen evolution reaction and electrocatalytic alcohol oxidation
- Synthesis of stable and selective electrocatalysts for CO_2 reduction for a closed carbon-cycle economy

Selected Publications

T. Tarnev, [...], C. Andronescu, W. Schuhman, Angew. Chem. Int. Ed. 58, 40 (2019).

D. Medina, S. Barwe, J. Masa, S. Seisel, W. Schuhmann, C. Andronescu, Electrochim. Acta 318, 281 (2019).

B. Alkan, S. Cychy, S. Varhade, M. Muhler, C. Schulz, W. Schuhmann, H. Wiggers, C. Andronescu, ChemElectroChem 6, 16 (2019).

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Research Topic

Chemical Vapor Deposition

- CVD of different materials (Al_2O_3, SiC, FeO, etc.)
- Process optimization
- Process diagnostics: mass spectrometry, laser diagnostics
- Precursor stability and precursor thermodynamics
- Combustion mechanisms

Selected Publications

B. Atakan, Energies 12, 17 (2019).

P. O. Oketch, M. Gonchikzhapov, U. Bergmann, B. Atakan, Measurement Science and Technology 30, 9 (2019).

D. Kaczmarek, B. Atakan, T. Kasper, Combustion Science and Technology 191, 9 (2019).

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Research Topic

Nanomaterials and Nano-devices

- Functionality of nanoscale materials and devices for micro-/optoelectronics
- Hybrid materials for spintronics – nanofabrication and analysis
- Quantum-dot based optoelectronics and quantum information technology

Selected Publications

F. Muckel, S. Delikanli, P. L. Hernandez-Martinez, T. Priesner, S. Lorenz, J. Ackermann, M. Sharma, H. V. Demir, G. Bacher, Nano Letters 18, 2047 (2018).

W.A. Quitsch, D. W. deQuilettes, O. Pfingsten, A. Schmitz, S. Ognjanovic, S. Jariwala, S. Koch, M. Winterer, D. S. Ginger, G. Bacher, J. Phys. Chem. Lett. 9, 2062 (2018).

O. Pfingsten, J. Klein, L. Protesescu, M. I. Bodnarchuk, M. V. Kovalenko, G. Bacher, Nano Letters 18, 4440 (2018).

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Research Topic

Laser-Generated Functional Nanoparticles and Materials

- Bioactive nanocomposites and bioconjugation of gold nanoparticles
- Nanoparticle polymer composites
- Dispersion and fragmentation of aggregates
- Synthesis of heterogeneous catalysts – supported particles

Selected Publications

A. Tymoczko, M. Kamp, O. Prymak, C. Rehbock, J. Jakobi, U. Schurmann, L. Kienle, S. Barcikowski, Nanoscale 10, 16434-16437 (2018).

S. Reichenberger, G. Marzun, M. Muhler, S. Barcikowski, ChemCatChem 11, 4489-4518 (2019).

A. Letzel, S. Reich, T. dos Santos Rolo, A. Kanitz, J. Hoppius, A. Rack, M. Olbinado, A. Ostendorf, B. Gökce, A. Plech, S. Barcikowski, Langmuir 35, 3038 (2019).

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Research Topic

Nanoporous Materials & their Industrial Application

- Adsorption in gas & liquid phase
- Environmental technology
- Energy technology

Selected Publications

F. Berg, C. Bläker, C. Pasel, M. Luckas, T. Eckhardt, D. Bathen, Microporous and Mesoporous Materials 264 (2018).

F. Birkmann, C. Pasel, M. Luckas, D. Bathen, Ind. & Eng, Chem. Res. 57, 23 (2018).

J. Ambrosy, C. Pasel, M. Luckas, M. Bittig, D. Bathen, Ind. & Eng. Chem. Res. 58, 10 (2019).

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Research Topic

Nanostructured Catalysts

- Nanoparticles on porous supports
- Catalytic CO_2 conversion
- Materials for water oxidation

Selected Publications

K. Chakrapani, G. Bendt, H. Hajiyani, T. Lunkenbein, M. T. Greiner, L. Masliuk, S. Salamon, J. Landers, R. Schlögl, H. Wende, R. Pentcheva, S. Schulz, M. Behrens, ACS Catalysis 8, 1259 (2018).

K. Chakrapani, F. Özcan, K. Friedel Ortega, T. Machowski, M. Behrens, ChemElectroChem 5, 93 (2018).

M. Rohloff, S. Cosgun, C. Massué, T. Lunkenbein, A. Senyshyn, M. Lerch, A. Fischer, M. Behrens, M., Z. Naturforsch. B 74, 71 (2019).

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Research Topic

Ultrafast Dynamics of Solids and their Interfaces

- Non-equilibrium states of correlated materials
- Electron relaxation in low dimensional structures
- Magnetism on ultrafast time scales

Selected Publications

T. Konstantinova, J. D. Rameau, A. H. Reid, O. Abdurazakov, L. Wu, R. Li, X. Shen, G. Gu, Y. Huang, L. Rettig, I. Avigo, M. Ligges, J. K. Freericks, A. F. Kemper, H. A. Dürr, U. Bovensiepen, P. D. Johnson, X. Wang, Y. Zhu, Sci. Adv. 4, 7427 (2018).

J. Chen, U. Bovensiepen, A. Eschenlohr, T. Müller, P. Elliott, E.K.U. Gross, J. K. Dewhurst, S. Sharma, Phys. Rev. Lett. 122, 067202 (2019).

V. Tinnemann, C. Streubühr, B. Hafke, A. Kalus, A. Hanisch-Blicharski, M. Ligges, P. Zhou, D. von der Linde, U. Bovensiepen, M. Horn-von Hoegen, Structural Dynamics 6, 035101 (2019).

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Research Topic

Functional Coatings

- Tribological coatings
- Biocompatible coatings
- Barrier coatings

Selected Publications

A. Giese, S. Schipporeit, V. Buck, N. Wöhrl, J. Beilstein, Nanotechnol. 9, 1895-1905 (2018).

T. Chakraborty, F. Lehmann, J. Zhang, S. Borgsdorf, N. Woehrl, R. Remfort, V. Buck, U. Köhler, D. Suter, Phys. Rev. Materials 3, 065205 (2019).

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Research Topic

Toxicity of Nanoparticles and Nanomaterials

- Cellular toxicity
- Genotoxicity in mammalian cells
- Extra- and intracellular radical formation

Selected Publications

L. Gehrmann, H. Bielak, M. Behr, F. Itzel, S. Lyko, A. Simon, G. Kunze, E. Dopp, M. Wagner, J. Türk, Environ Sci Pollut Res 26, 15724 (2019).

E. Dopp, H. Pannekens, F. Itzel, J. Türk, International Journal of Hygiene and Environmental Health 222, 607 (2019).

H. Pannekens, A. Gottschlich, H. Hollert, E. Dopp, International Journal of Hygiene and Environmental Health 222, 670 (2019).

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Research Topic

Laser-based gas phase and aerosol diagnostics

- Laser-induced fluorescence (LIF) of tracer species
- Laser diagnostics in nanoparticle pilot plants
- Laser-induced incandescence (LII) of metal and metal oxide nanoparticles
- Chemiluminescence in flames and plasmas

Selected Publications

K. Daun, J. Menser, M. Asif, S. Musikhin, T. Dreier, C. Schulz, J. Quant. Spectrosc. Radiat. Transf. 226, 146 (2019).

R. S. M. Chrystie, H. Janbazi, T. Dreier, H. Wiggers, I. Wlokas, C. Schulz, Proc. Combust. Inst. 37, 1221 (2019).

C. Schulz, T. Dreier, M. Fikri, H. Wiggers, Proc. Combust. Inst. 37, 83 (2019).

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Research Topic

Many-Particle Physics and First-Principles Methods

- Large-scale molecular dynamics and ab initio simulations
- Correlated electron systems
- Electric transport in heterostructures

Selected Publications

P. Entel, M. E. Gruner et al., Physica Status Solidi B 255, 2 (2018).

V. Popescu, P. Kratzer, P. Entel et al., Journal of Physics D: Applied Physics 52, 7 (2019).

V. V. Sokolovskiy, M. E. Gruner, P. Entel, M. Acet, A. Çakır, D. R. Baigutlin, V. D. Buchelnikov, Physical Review Materials 3, 8 (2019).

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Research Topic

Nanobiomedicine

- Nanoparticles for medical application
- Nanocomposites for heterogeneous catalysis
- Nanocrystalline ceramics for biomedicine

Selected Publications

V. Grasmik, C. Rurainsky, K. Loza, M.V. Evers, O. Prymak, M. Heggen, K. Tschulik, M. Epple, Chem. Eur. J. 24, 9051 (2018).

M. Epple, Acta Biomater. 77, 1 (2018).

S. B. van der Meer, K. Loza, K. Wey, M. Heggen, C. Beuck, P. Bayer, M. Epple, Langmuir 35, 7191 (2019).

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Research Topic

Computational Nanophotonics and Nanoelectromagnetics

- Electromagnetic and optical metamaterials
- Plasmonics and optical antennas
- Nanophotonics and optical interconnects
- Full-wave modelling and numerical structural optimization

Selected Publications

V. Jandieri, R. Khomeriki, D. Erni, Opt. Express 26, 16 (2018).

V. Tran, C. Thiel, J. T. Svejda, M. Jalali, B. Walkenfort, D. Erni, S. Schluecker, Nanoscale 10, 46 (2018).

M. Jalali, T. Jalali, H. Nadgaran, D. Erni, J. Opt. Soc. Am. B 36, 1 (2019).

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Research Topic

Nanomagnetism

- Magnetic, electronic and crystal structure of nanocrystals and ultrathin films
- Fundamental interactions, spin dynamics and spin transport
- Functionalization and hybrid nanomagnets

Selected Publications

T. Marzi, R. Meckenstock, S. Masur, M. Farle, Physical Review Applied 10, 5 (2018).

Q. Tao, J. Lu, M. Dahlqvist, A. Mockute, S. Calder, A. Petruhins, R. Meshkian, O. Rivin, D. Potashnikov, E. a. N. Caspi, H. Shaked, A. Hoser, C. Opagiste, R.-M. Galera, R. Salikhov, U. Wiedwald, C. Ritter, A. R. Wildes, B. Johansson, L. Hultman, M. Farle, M. W. Barsoum, J. Rosen, Chem Mater 31, 2476-2485 (2019).

B. W. Zingsem, M. Farle, R. L. Stamps, R. E. Camley, Physical Review B 99, 214429 (2019).

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Research Topic

Synthesis, characterization and use of perfluorocarbon-based artificial oxygen carriers (AOCs)

- Perfluorocarbon-based AOCs as blood substitutes
- Perfluorocarbon-based AOCs to improve quality of organs prior to transplantation
- Treatment of decompression sickness with perfluorocarbon-based AOCs

Selected Publications

J. Köhler, J. Ruschke, K. B. Ferenz, C. Esen, M. Kirsch, A. Ostendorf, Biomed Opt Exp 9, 743-754 (2018).

K. B. Ferenz, A. Steinbicker, J Pharmacol Exp Ther 369, 300-10 (2019).

K. B. Ferenz, Elsevier (2019) (ISBN: 9780128142257, in press).

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Research Topic

High-temperature kinetics in shock-wave and flow reactors

- Studies of elementary reactions
- Combustion and ignition processes
- Mass spectrometric and laser-based diagnostics in pyrolytic and oxidative systems

Selected Publications

C. Schulz, T. Dreier, M. Fikri, H. Wiggers, Proceedings of the Combustion Institute 37, 1 (2019).

P. Sela, Y. Sakai, H. S. Choi, J. Herzler, M. Fikri, C. Schulz, S. Peukert, Journal of Physical Chemistry A 123, 32 (2019).

P. Sela, S. Peukert, J. Herzler, Y. Sakai, M. Fikri, C. Schulz, Proceedings of the Combustion Institute 37, 1 (2019).

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Research Topic

Sustainable Nanotechnology – Nanoparticle Exposure

- Development of measurement devices and exposure measurement strategies
- Nanoparticle fate after release
- Dosis determination for human beings and environment

Selected Publications

S.-C. Chen, J. Wang, H. Fissan, D. Y. H. Pui, Aerosol Science and Technology 49, 8 (2015).

L. N. Y. Cao, S.-C. Chen, H. Fissan, C. Asbach, D. Y. H. Pui, J. Aerosol Sci. 114 (2017).

T. Hammera, H. Fissan, J. Wang, NanoImpact 14 (2019).

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Research Topic

Optical and Transport Properties of Nanostructures

- Transport measurements on low-dimensional quantum systems (quantum dots, two-dimensional electron gases)
- Interaction between nanoobjects
- Optical spectroscopy on nanoparticles/quantum dots
- Nanopatterning techniques (focused ion beam, electron beam lithography)

Selected Publications

A. Kurzmann, P. Stegmann, J. Kerski, R. Schott, A. Ludwig, A. D. Wieck, J. Koenig, A. Lorke, M. Geller, Phys. Rev. Lett. 122, 247403 (2019).

P. Lochner, A. Kurzmann, R. Schott, A. D. Wieck, A. Ludwig, A. Lorke, M. Geller, Scientific Reports 9, 8817 (2019).

A. Al-Ashouri, A. Kurzmann, B. Merkel, A. Ludwig, A. D. Wieck, A. Lorke, M. Geller, Nano Letters 19, 135 (2019).

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Research Topic

Supramolecular Materials

- Supramolecular liquid crystals
- Photo-responsive materials
- Synthesis of photonic nanostructures
- Photonic sensors

Selected Publications

M. Spengler, R. Y. Dong, C. A. Michal, W.Y. Hamad, M. J. MacLachlan, M. Giese, Adv. Funct. Mater. 28, 1800207-1800207 (2018).

M. Saccone, M. Spengler, M. Pfletscher, K. Kuntze, M. Virkki, C. Wölper, R. Gehrke, G. Jansen, P. Metrangolo, A. Priimagi, M. Giese, Chem. Mater. 31, 461-470 (2019).

M. Saccone, M. Pfletscher, E. Dautzenberg, R. Y. Dong, C. A. Michal, M. Giese, J. Mater. Chem. C 7, 3150-3153 (2019).

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Research Topic

Laser-Based Nanomaterials

- Synthesis of magnetic, optically active and alloy nanoparticles
- Application of nanomaterials in optics, electronics, photocatalysis and tribology
- Physical fundamentals and upscaling of laser-based nanoparticle synthesis

Selected Publications

C. Doñate-Buendía, F. Frömel, M. B. Wilms, R. Streubel, J. Tenkamp, T. Hupfeld, M. Nachev, E. Gökce, A. Weisheit, S. Barcikowski, F. Walther, J. H. Schleifenbaum, B. Gökce, Materials & Design 154, 360 (2018).

F. Waag, Y. Li, A. Ziefuß, E. Bertin, M. Kamp, V. Duppel, G. Marzun, L. Kienle, S. Barcikowski, B. Gökce, RSC Advances 9, 18547 (2019).

S. Jendrzej, L. Gondecki, J. Debus, H. Moldenhauer, P. Tenberge, S. Barcikowski, B. Gökce, Applied Surface Science 467, 811 (2019).

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Research Topic
Colloid and Polymer Science

- Synthesis of functional polymers and complex polymer architectures
- Self-assembly of block copolymer and nanoparticles
- Hierarchical mesostructures
- Organic supports and nanocomposites
- Polymer processing

Selected Publications

M. Poutanen, G. Guidetti, T. I. Gröschel, O. Borisov, S. Vignolini, O. Ikkala, A. H. Gröschel, ACS Nano 12, 3149 (2018).

A. Steinhaus, R. Chakroun, T.-L. Nghiem, M. Müllner, M. Hildebrandt, A.H. Gröschel, ACS Nano 13, 6269 (2019).

X. Qiang, A. Steinhaus, R. Chakroun, C. Chen, A. H. Gröschel, Angew. Chem. Int. Ed. 21, 7122 (2019).

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Research Topic
Ab initio simulations of functional magnetic materials

- Energy conversion materials: shape memory alloys and magnetocaloric effect
- Competion of magnetic and elastic interactions: Lattice dynamics and martensitic microstructure on the nanoscale
- Metallic nanoparticles: Structural stability, spin and orbital magentism

Selected Publications

A. Waske, M. E. Gruner, T. Gottschall, O. Gutfleisch, MRS Bulletin 43, 269 (2018).

M. E. Gruner, R. Niemann, P. Entel, R. Pentcheva, U. K. Rössler, K. Nielsch, S. Fähler, Scientific Reports 8, 8489 (2018).

M. E. Gruner, R. Pentcheva, Phys. Rev. B 99, 195104 (2019).

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Research Topic
Nanostructured Thin Films

- Synthesis of functional polymer coatings
- Microcantilever sensors
- Grazing incidence scattering techniques

Selected Publications

W. Ali, B. Gebert, S. Altinpinar, T. Mayer-Gall, M. Ulbricht, J. S. Gutmann, K. Graf, Polymers 10, 567 (2018).

L. M. Timma, L. Lewald, F. Gier, L. Homey, C. Neyer, A. Nichisch-Hartfiel, J. S. Gutmann, M. Oberthür, RSC Advances 9, 9783 (2019).

W. Ali, V. Shabani, M. Linke, S. Sayin, B. Gebert, S. Altinpinar, M. Hildebrandt, J. S. Gutmann, T. Mayer-Gall, RSC Advances 9, 4553 (2019).

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Research Topic
Metallurgical Mechanisms of Cyclic and Monotonic Deformation

- Dynamic recrystallization and grain refining
- Relation of micro-/nanostructure and damage mechanisms due to sliding wear, cavitation and fatigue of metallic materials
- Dynamic recrystallization and material behavior during friction surfacing and friction stir welding

Selected Publications

H. J. Sagar, S. Hanke, M. Underberg, C. Feng, O. el Moctar, S. A. Kaiser, Mater. Perform. Charact. 7, 985-1003 (2018).

M. Abedini, F. Reuter, S. Hanke, Ultrason. Sonochem. 58, 104628 (2019).

H. M. Sajjad, S. Hanke, S. Güler, H. ul Hassan, A. Fischer, A. Hartmaier, Materials 12, 1767 (2019).

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Research Topic

Surface Dynamics

- Nanostructuring of surfaces for functionalization with organic monolayers
- Gas-surface dynamics & surface photochemistry
- Time-resolved dynamics of vibrations at surfaces

Selected Publications

M. Lackner, D. Lucaßen, E. Hasselbrink, Chem. Phys. Lett. 713, 277 (2018).

J. P. Meyburg, D. Diesing, E. Hasselbrink, Surf. Sci 678, 91 (2018).

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Research Topic

Fuel Cell Technology

- Membrane fuel cells, micro fuel cells
- Hydrogen generation and storage
- Electrochemistry and surfaces

Selected Publications

U. Misz, A. Talke, A. Heinzel, P. Beckhaus, 6th European PEFC & Electrolyzer Forum (2018).

A. Heinzel, M. Cappadonia, U. Stimming, K.V. Kordesch, J. C. T. Oliveira, Ullmann´s Encyclopedia of Industrial Chemistry Online (2018).

S. Gößling, S. Stypka, B. Oberschachtsiek, M. Bahr, A. Heinzel, Chemie Ingenieur Technik, 90, 1437 (2018).

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Research Topic

Morphology and Dynamics of Surfaces

- Manipulation of semiconductor surface morphology
- Epitaxial growth, surfactant mediated epitaxy
- Selforganization of nanostructures
- Ultrafast electron and lattice dynamics in nanostructures

Selected Publications

M. Horn von Hoegen, MRS Bulletin 43, 512-519 (2018).

K. M. Omambac, H. Hattab, C. Brand, G. Jnawali, A. T. N'Diaye, J. Coraux, R. van Gastel, B. Poelsema, T. Michely, F.-J. Meyer zu Heringdorf, M. Horn-von Hoegen, Nano Letters 19, 4594 (2019).

D. Meyer, G. Jnawali, H. Hattab, M. Horn-von Hoegen, Applied Physics Letters 114, 081601 (2019).

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Research Topic

Fluctuation-induced interactions in and out of equilibrium

- Critical behavior
- Universal scaling functions
- Colloids in binary liquids
- Cluster Monte Carlo methods

Selected Publications

A. Hucht, J. Phys. A: Math. Theor. 50, 065201 (2017).

A. Hucht, J. Phys. A: Math. Theor. 50, 265205 (2017).

A. Kundu, M. E. Gruner, M. Siewert, A. Hucht, P. Entel, S. Ghosh, Phys. Rev. B 96, 064107 (2017).

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Research Topic

Mass Spectrometry in Reacting Flows

- Mass spectrometry diagnostics in energy transformation processes
- Combustion chemistry of prototypical biofuels
- Mass spectrometry system for diagnostic in flames

Selected Publications

Y. Karakaya, S. Peukert, T. Kasper, Journal of Physical Chemistry A 122, 7131-7141 (2018).

D. Kaczmarek, B. Atakan, T. Kasper, Combustion and Flame 205, 345-357 (2019).

D. Krüger, P. Oßwald, M. Köhler, P. Hemberger, T. Bierkandt, T. Kasper, Proceedings of the Combustion Institute 37, 1563-1570 (2019).

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Research Topic

Simulation of Reactive Flows

- Nano-particle synthesis
- Multi scale modelling
- Chemical mechanisms
- Turbulent combustion
- Large eddy simulation

Selected Publications

H. Janbazi, O. Hasemann, C. Schulz, A. M. Kempf, I. Wlokas, S. Peukert, Int. J. Chem. Kinet. 1–10 (2018).

L. Cifuentes, A. M. Kempf, C. Dopazo, Proc. Comb. Inst. (2018).

J. T. Lipkowicz, I. Wlokas, A. M. Kempf, Shock Waves 1-11 (2018).

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Research Topic

Thin-Film Photovoltaics

- Organic and hybrid photovoltaics
- Electrical characterization and simulation of solar cells
- Electroluminescence as characterization tool for solar cells

Selected Publications

T. Kirchartz, U. Rau., Adv. Energy Mater. 8, 1703385 (2018).

J. F. Guillemoles, T. Kirchartz, D. Cahen, U. Rau., Nature Photonics 13, 501 (2019).

T. Kirchartz, Phil. Trans. R. Soc. A 377, 20180286 (2019).

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Research Topic

Nanobiomedicine

- Therapeutic application of nanoparticles
- Intracellular transport of nanoparticles
- Nanoparticle protein corona

Selected Publications

D. Westmeier, D. Solouk-Saran, C. Vallet, S. Siemer, D. Docter, H. Gotz, L. Mann, A. Hasenberg, A. Hahlbrock, K. Erler, C. Reinhardt, O. Schilling, S. Becker, M. Gunzer, M. Hasenberg, S. K. Knauer, R. H. Stauber, Proc Natl Acad Sci USA 115, 7087-7092 (2018).

S. Siemer, D. Westmeier, C. Vallet, J. Steinmann, J. Buer, R. H. Stauber, S. K. Knauer, Materials Today 26, 19-29 (2018).

R. H. Stauber, S. Siemer, S. Becker, G. B. Ding, S. Strieth, S. K. Knauer, ACS Nano 12, 6351-6359 (2018).

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Research Topic

Condensed Matter Theory

- Quantum transport in nano-structures
- Spintronics
- Diagrammatic transport theory

Selected Publications

E. Kleinherbers, P. Stegmann, J. König, New J. Phys. 20, 073023 (2018).

A. Kurzmann, P. Stegmann, J. Kerski, R. Schott, A. Ludwig, A. D. Wieck, J. König, A. Lorke, M. Geller, Phys. Rev. Lett. 122, 247403 (2019).

S. Mundinar, P. Stegmann, J. König, S. Weiss, Phys. Rev. B 99, 195457 (2019).

Prof. Dr. Peter Kratzer
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Research Topic

First-Principles and Statistical Methods in Materials Physics

- Ab initio theory of elementary excitations at surfaces
- Atomic and electronic structure of thin magnetic films
- Growth simulations of semiconductor quantum dots and quantum wires
- Thermoelectric properties of self-assembled nanocrystals in a semiconductor matrix
- Spincaloritronics in alloy heterostructures

Selected Publications

A. U. Rahman, J. M. Morbec, G. Rahman, P. Kratzer, Phys. Rev. Mat. 2, 094002 (2018).

H. Kahnouji, P. Kratzer, S. J. Hashemifar, Phys. Rev. B 99, 035418 (2019).

B. Geisler, P. Kratzer, Phys. Rev. B 99, 155433 (2019).

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Research Topic

Nanoparticles, Nanoaerosols and Nanoparticulate Layers

- Gas-phase synthesis of nanoparticles, especially by means of electrical discharges
- Technology for size-selection and deposition
- Modeling of dynamic behavior and transport of nanoaerosols, especially by means of Monte Carlo simulations
- Functional thin films, e.g. gas sensors or nanoparticle-reinforced coatings

Selected Publications

M. Stein, F. E. Kruis, Advanced Powder Technology 29, 3138 (2018).

D. Kiesler, T. Bastuck, M. K. Kennedy, F. E. Kruis, Aerosol Science and Technology 53, 630 (2019).

G. Kotalczyk, I. Skenderovic, F. E. Kruis, Tellus, Series B: Chemical and Physical Meteorology 71, 1 (2019).

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Research Topic

Nanoparticles - Mobility, Exposure and Effects

- Sustainable nanotechnology
- Development of measurement techniques and devices
- Modelling and measurements for exposure assessments
- Mobility studies of nano-objects for lifecycle and risk assessments

Selected Publications

R. Hebisch, T. A. J. Kuhlbusch, K. Bux, D. Breuer, T. Lahrz, Gefahrstoffe, Reinhaltung der Luft 79, 255 (2019).

W. Wohlleben, H. Brian, C. Nickel, M. Herrchen, K. Hund-Rinke, K. Kettler, C. Riebeling, A. Haase, B. Funk, D. Kühnel, D. Göhler, M. Stintz, C. Schumacher, M. Wiemann, J. Keller, R. Landsiedel, D. Broßell, S. Plitzko, T. A. J. Kuhlbusch, Nanoscale 11, 17637 (2019).

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Research Topic

Optoelectronic Devices based on Nanostructures

- Nanoparticle, nanowire and quantum dot light emitters
- Control of single spins and charges in quantum structures
- Top-down nanofabrication using electron beam lithography

Selected Publications

D. Andrzejewski, M. Marx, A. Grundmann, O. Pfingsten, H. Kalisch, A. Vescan, M. Heuken, T. Kümmell, G. Bacher, Nanotechnology 29, 295704 (2018).

D. Andrzejewski, E. Hopmann, M. John, T. Kümmell, G. Bacher, Nanoscale 11, 8372 (2019).

D. Andrzejewski, H. Myja, M. Heuken, A. Grundmann, H. Kalisch, A. Vescan, T. Kümmell, G. Bacher, ACS Photonics 6, 1832-1839 (2019).

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Research Topic

Semiconductors and Nanostructures

- Quantum dots, ballistic and quantum transport
- Self-organized nanostructures
- Optical-spectroscopy

Selected Publications

M. F. Linder, A. Lorke, R. Schützhold, Phys. Rev. B 97, 035203 (2018).

A. Kurzmann, P. Stegmann, J. Kerski, R. Schott, A. Ludwig, A. D. Wieck, J. Koenig, A. Lorke, M. Geller, Phys. Rev. Lett. 122, 247403 (2019).

A. Al-Ashouri, A. Kurzmann, B. Merkel, A. Ludwig, A. D. Wieck, A. Lorke, M. Geller, Nano Letters 19, 135 (2019).

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Research Topic

Functional Materials

- Ferroelectric, piezoelectric, magnetoelctric materials and realxors for actuator and sensor applications (nano to macro)
- Organic hybrid photovoltaic and photocatalysis
- Mechanics of functional materials (nano to macro)
- Nanothermoisolation

Selected Publications

J. Schell, D. V. Zyabkin, D. C. Lupascu, H. Hofsäss, M. O. Karabasov, A. Welker, P. Schaaf, AIP Advances 9, 8 (2019).

D. Ganter, T. Mielke, M. Maier, D. C. Lupascu, Construction and Building Materials 222 (2019).

J. Schell, H. Hofsäss, D. C. Lupascu, Nuclear Instruments and Methods in Physics Research B: Beam Interactions with Materials and Atoms (2019).

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Research Topic

Nanoparticles and Nanocapsules based on Organic Matrices

- Synthesis and analysis of polymer nanocapsules and vesicles
- Nuclear magnetic resonance (NMR), especially solid state NMR and pulsed field gradient NMR

Selected Publications

Y. Xiong, D. Gu, X. Deng, H. Tüysüz, M. van Gastel, F. Schüth, F. Marlow, Microporous and Mesoporous Materials 268, 162 (2018).

S. Abdellatif, S. Josten, P. Sharifi, K. Kirah, R. Ghannam, A. S. G. Khalil, D. Erni, F. Marlow, Proc. SPIE 10526, 105260A1 (2018).

S. Abdellatif, P. Sharifi, K. Kirah, R. Ghannam, A. Khalil, D. Erni, F. Marlow, Microporous and Mesoporous Materials 264, 84 (2018).

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Research Topic

Nanoparticles and Nanocapsules based on Organic Matrices

- Synthesis and analysis of polymer nanocapsules and vesicles
- Nuclear magnetic resonance (NMR), especially solid state NMR and pulsed field gradient NMR

Selected Publications

S. M. Ognjanovic, M. Zähres, C. Mayer, M. Winterer, J. Phys. Chem. 122, 23749 (2018).

C. Mayer, U. Schreiber, M. J. Davila, O. J. Schmitz, A. Bronja, M. Meyer, J. Klein, S. W. Meckelmann, Life 8, 16 (2018).

T. Ruks, C. Beuck, T. Schaller, F. Niemeyer, M. Zähres, K. Loza, M. Heggen, U. Hagemann, C. Mayer, P. Bayer, M. Epple, Langmuir 35, 767 (2019).

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Research Topic

Electrical Nanoanalytics

- Nanocharacterization of micro-/optoelectronic materials and devices
- Kelvin probe force microscopy

Selected Publications

M. Shaygan, M. Otto, A. A. Sagade, C. A. Chavarin, G. Bacher, W. Mertin, D. Neumaier, Ann. Phys. (Berlin) 1600410 (2017).

B. Bekdüz, L. Kampermann, W. Mertin, C. Punckt, I. A. Aksay, G. Bacher, RSA Advances 8, 42073 (2018).

B. Bekdüz, Y. Beckmann, J. Mischke, J. Twellmann, W. Mertin, G. Bacher, Nanotechnology 29, 455603 (2018).

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Research Topic

In-Situ Surface Microscopy

- Low energy electron microscopy and time-resolved photoemission electron microscopy
- Self-assembly of nanostructures
- Plasmon dynamics in a semiconductor matrix
- Organic thin films and devices

Selected Publications

P. Kahl, D. Podbiel, C. Schneider, A. Makris, S. Sindermann, C. Witt, D. Kilbane, M. Horn-von Hoegen, M. Aeschlimann, F. Meyer zu Heringdorf, Plasmonics 13, 239-246 (2018).

D. Podbiel, P. Kahl, B. Frank, T. J. Davis, H. Giessen, M. Horn-von Hoegen, F. Meyer zu Heringdorf, ACS Photonics Jg. 6, 600 - 604 (2019).

K. Omambac, H. Hattab, C. Brand, G. Jnawali, A. T. N'Diaye, J. Coraux, R. van Gastel, B. Poelsema, T. Michely, F. Meyer zu Heringdorf, M. Horn-von Hoegen, Nano Letters 19, 4594-4600 (2019).

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Research Topic

Interfaces on the Atomic Scale

- Analysis of organic monolayers on metallic, semi conducting and insulating surfaces
- Elementary processes of friction and energy dissipation
- Electronic transport

Selected Publications

P. Graf, M. Flebbe, S. Hoepken, D. Utzat, H. Nienhaus, R. Möller, Applied Physics Letters 113, 223101 (2018).

E. Genc, A. Mölleken, D. Tarasevitch, D. Utzat, H. Nienhaus, R. Möller, Rev. Sci. Instrum. 90, 075115 (2019).

A. Kavangary, P. Graf, H. Azazoglu, M. Flebbe, K. Huba, H. Nienhaus, R. Möller, AIP Advances 9, 025104 (2019).

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Research Topic

Functional Supramolecular Systems

- Synthesis of interlocked molecules (catenanes, rotaxanes)
- Formation of molecular capsules and helical structures by self-aggregation
- Host/guest-chemistry and catalysis

Selected Publications

F. Octa-Smolin, F. van der Vight, R. Yadav, J. Bhangu, K. Soloviova, C. Wölper, C. G. Daniliuc, C. Strassert, H. Somnitz, G. Jansen, J. Niemeyer, J. Org. Chem. 83, 14568 (2018).

F. Octa-Smolin, J. Niemeyer, Chem. Eur. J. 24, 16506 (2018).

M. Kohlhaas, M. Zähres, C. Mayer, M. Engeser, C. Merten, J. Niemeyer, Chem. Commun. 55, 3298 (2019).

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Research Topic

Reactions at Surfaces and Nanostructures

- Chemically induced electronic excitations
- Chemiluminescence
- Vibrational, electronic and chemical properties of surfaces, interfaces and nanoparticles
- Chemical sensing with electronic devices

Selected Publications

U. Hagemann, K. Huba, H. Nienhaus, J. Appl. Phys. 124, 225302 (2018).

P. Graf, M. Flebbe, S. Hoepken, D. Utzat, H. Nienhaus, R. Möller, Appl. Phys. Lett. 113, 223101 (2018).

E. Genc, A. Mölleken, D. Tarasevitch, D. Utzat, H. Nienhaus, R. Möller, Rev. Sci. Instrum. 90, 075115 (2019).

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Research Topic

Computational Material Physics

- Nanoscaled oxides for electronics, spintronics, and energy conversion
- Boundary surface induced electronic phenomena
- Topological nontrivial phases

Selected Publications

H. Hajiyani, R. Pentcheva, ACS Catal. 8, 11773-11782 (2018).

B. Geisler, R. Pentcheva, Phys. Rev. Applied 11, 044047 (2019).

M. E. Gruner, R. Pentcheva, Phys. Rev. B 99, 195104 (2019).

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Research Topic

III/V Semiconductor Heterostructures

- Nanowire photonics
- Nanoelectronic circuits
- Tunneling diodes

Selected Publications

S. Heedt, N. T. Ziani, F. Crépin, W. Prost, S. Trellenkamp, J. Schubert, D. Grützmacher, B. Trauzettel, T. Schäpers, Nature Physics 13, 563–567 (2017).

C. Blumberg, S. Grosse, N. Weimann, F.-J. Tegude, W. Prost, Physica Status Solidi B 255, 1700485 (2018).

K. Arzi, S. Clochiatti, S. Suzuki, A. Rennings, D. Erni, N. Weimann, M. Asada, W. Prost, Proc. GeMiC (2019).

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Research Topic

Bionanotechnology

- Design and self-assembly of DNA nanostructures by structural DNA nanotechnology (multi-stranded and DNA origami methods)
- Development of DNA-based nanocontainers for confined chemical reactions
- Development of switchable DNA-based nanodevices for spatio-temporal control of biochemical processes

Selected Publications

A. Sprengel, P. Lill, P. Stegemann, K. Bravo-Rodriguez, E. Schöneweiß, M. Merdanovic, D. Gudnason, M. Aznauryan, L. Gamrad, S. Barcikowski, E. Sanchez-Garcia, V. Birkedal, C. Gatsogiannis, M. Ehrmann, B. Saccà, Nat Commun. 8, 14472 (2017).

W. Pfeifer, P. Lill, C. Gatsogiannis, B. Saccà, ACS Nano, 12, 44 (2018).

R. Kosinski, A. Mukhortava, W. Pfeifer, A. Candelli, P. Rauch, B. Saccà, Nat. Commun. 10, 1 (2019).

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Research Topic

Modification of Surfaces and Nanostructures

- Nanoscaled modifications by energetic ions
- Electronic conductivity of metallic nanostructures
- Dynamic force microscopy
- Graphs and 2D materials

Selected Publications

L. Madauß, [...], B. Roldan Cuenya, M. Schleberger, Nanoscale 10, 22908 (2018).

R. Kozubek, P. Ernst, C. Herbig, T. Michely, M. Schleberger, ACS Applied Nano Materials 1, 3765 (2018).

R. Kozubek, M. Tripathi, M. Ghorbani-Asl, S. Kretschmer, L. Madauß, E. Pollmann, M. O´Brien, N. McEvoy, U. Ludacka, T. Susi, G. Duesberg, R. A. Wilhelm, A. V. Krasheninnikov, J. Kotakoski, M. Schleberger, J. Phys. Chem. Lett. 10, 904 (2019).

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Research Topic

Nano Bio Photonics

- Nano particle label reagents: design, synthesis and physical properties of SERS nano particles with defined geometries
- Nano bio photonics: tissue based tumor diagnostics using immune SERS microscopy
- Nano bio analytics: development of nano particle based assays for high sensitive detection of biological targeting molecule

Selected Publications

V. Tran, B. Walkenfort, M. König, M. Salehi, S. Schlücker, Angew. Chem. Int. Ed. 58, 442 (2019).

J. H. Yoon, F. Selbach, L. Langolf, S. Schlücker, Small 14, 1702754 (2018).

Y. Zhang, X. Wang, S. Perner, A. Bankfalvi, S. Schlücker, Anal. Chem. 90, 760 (2018).

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Research Topic

Functional Nanoparticulate Layers and Organic/Inorganic Nanocomposites for Electronic Applications

- Printable Electronics
- Photovoltaic
- Thermoelectric

Selected Publications

R. Chavez, S. Angst, J. Hall, F. Maculewicz, J. Stötzel, H. Wiggers, L T. Hung, N. V. Nong, N. Pryds, G. Span, D. E. Wolf, R. Schmechel, G. Schierning, J. Phys. D: Appl. Phys. 51, 014005 (2018).

F. Maculewicz, T. Wagner, K. Arzi, N. Hartmann, N. Weimann, R. Schmechel, J. Appl. Phys. 125, 184502 (2019).

K. Rojek, R. Schmechel, N. Benson, Applied Physics Letters 114, 152104 (2019).

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Research Topic

Multi-optical concepts for solar energy

- Chalcopyrite-based photovoltaics
- Nano and micro structures for light guiding
- Multi-physics simulations

Selected Publications

F. Ringleb, S. Andree, B. Heidmann, J. Bonse, K. Eylers, O. Ernst, T. Boeck, M. Schmid, J. Krüger, Beilstein Journal of Nanotechnology 9, 3025 (2018).

P. Manley, F. F. Abdi, S. Berglund, A. T. M. N. Islam, S. Burger, R. van de Krol, M. Schmid, ACS Applied Energy Materials 1, 5810 (2018).

G. Yin, M. Song, M. Schmid, Solar Energy Materials and Solar Cells 195, 318 (2019).

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Research Topic

Aerosol Technology and Filtration

- Particle and gas phase filtration
- Functionalization of filter media and nanoporous materials
- Transport and deposition of (nano)particles

Selected Publications

R. Ligotski, U. Sager, U. Schneiderwind, C. Asbach, F. Schmidt, Building and Environment 149 (2019).

F. Schmidt, J. Weimann, C. König, Gefahrstoffe – Reinhaltung der Luft 79 (2019).

F. Schmidt, E. Däuber, T. Schuldt, T. Engelke, Filtrieren und Separieren 33 (2019).

Prof. Dr. Carsten Schmuck (†)
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Research Topic

Supramolecular Self-Assembly

- Synthesis and characterization of self-assembling zwitterions
- Formation of nanoparticles such as vesicles or monolayers in polar solvents and on surfaces
- Supramolecular polymers based on ionpair formation and metal-ligand interactions

Selected Publications

M. T. Fenske, W. Meyer-Zaika, H.-G. Korth, H. Vieker, A. Turchanin and C. Schmuck, J. Am. Chem. Soc. 135, 8342-8349 (2013).

M. Li, M. R. Stojkovic, M. Ehlers, E. Zellermann, I. Piantanida, C. Schmuck, Angewandte Chemie International Edition 55, 42 (2016).

J. Hatai, C. Schmuck, Acc. Chem. Res. 52, 1709-1720 (2019).

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Research Topic

Electronic Structure and Properties of Solids

- Magnetism in reduced dimensions
- Spintronics and spin-dependent transport phenomena
- Magnetization and spin dynamics
- Synchrotron-radiation based analytics

Selected Publications

C. Tusche, M. Ellguth, V. Feyer, A. Krasyuk, C. Wiemann, J. Henk, C. M. Schneider, J. Kirschner, Nat. Comm. 9, 3727 (2018).

S.-G. Gang, R. Adam, M. Plötzing, M. v. Witzleben, C. Weier, U. Parlak, D. Bürgler, P. Maldonado, J. Rusz, P. M. Oppeneer, C. M. Schneider, Phys. Rev. B 97, 064412 (2018).

E. Młynczak, M. C. T. D. Müller, P. Gospodaric, T. Heider, I. Aguilera, M. Gehlmann, M. Jugovac, G. Zamborlini, C. Tusche, S. Suga, V. Feyer, L. Plucinski, C. Friedrich, S. Blügel, C. M. Schneider, Nat. Comm. 10, 505 (2019).

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Research Topic

Reactive Flows

- Synthesis of nanoparticles from the gas phase
- Laser-based gas-phase and aerosol diagnostics
- Combustion and ignition processes
- High-temperature chemical kinetics
- Internal combustion engines

Selected Publications

A. Münzer, L. Xiao, Y. H. Sehlleier, C. Schulz, H. Wiggers, Electrochim. Acta 272, 52 (2018).

C. Schulz, T. Dreier, M. Fikri, H. Wiggers, Proc. Combust. Inst. 37, 83 (2019).

K. J. Daun, J. Menser, M. Asif, S. Musikhin, T. Dreier, C. Schulz, J. Quant. Spectrosc. Rad. Transf. 226, 146-156 (2019).

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Research Topic

Thin Films and Nanoparticles

- Synthesis of organometallic tailor-made precursors for metals and semiconductors
- Thin film deposition by MOCVD process
- Size- and shape-selective synthesis of nanoparticles in solution

Selected Publications

C. Ganesamoorthy, C. Helling, C. Wölper, W. Frank, E. Bill, G. E. Cutsail III, S. Schulz, Nat. Commun. 9, 87 (2018).

C. Helling, C. Wölper, S. Schulz, J. Am. Chem. Soc. 140, 5053 (2018).

G. Bendt, K. Kaiser, A. Heckel, F. Rieger, D. Oing, A. Lorke, N. Perez Rodriguez, G. Schierning, C. Jooss, S. Schulz, Semicond. Sci. Technol. 33, 105002 (2018).

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Research Topic

Heterogeneous Catalysis

- Synthesis and properties of porous nanostructures
- Hydrogen storage
- Biomass conversion

Selected Publications

J. Knossalla, P. Paciok, D. Gohl, D. Jalalpoor, E. Pizzutilo, A. M. Mingers, M. Heggen, R. E. Dunin-Borkowski, K. J. J. Mayrhofer, F. Schüth, J. Am. Chem. Soc., 15684 (2018).

H. Schreyer, R. Eckert, S. Immohr, J. de Bellis, M. Felderhoff, F. Schüth, Angw. Chem., Int. Ed., 11262 (2019).

M. Bilke, P. Losch, O. Vozniuk, A. Bodach, F. Schüth, J. Am. Chem. Soc., 141, 11212 (2019).

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Research Topic

Particle Technology

- Characterization of colloidal interfaces
- Formulation of funtional nano-materials
- Scalable, roll-to-roll printing technologies

Selected Publications

W. Lin, J. Schmidt, M. Mahler, T. Schindler, T. Unruh, B. Meyer, W. Peukert and D. Segets, Langmuir 33, 13581-13589 (2017).

S. Süß, T. Sobisch, W. Peukert, D. Lerche, D. Segets, Advanced Powder Technology 29, 7 (2018).

C. Menter, S. Segets, Advanced Powder Technology (2019).

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Research Topic

Ultrafast Dynamics in Laser-Driven Materials

- Structural dynamics in laser-excited solids and nanostructures
- Ultrafast phase transitions and laser ablation
- Femtosecond X-ray science

Selected Publications

M. Z. Mo, [...], K. Sokolowski-Tinten, Y. Y. Tsui, Y. Q. Wang, Q. Zheng, X. J. Wang, S. H. Glenzer, Science 360, 1451 (2018).

L. Schumacher, [...], F. Meyer zu Heringdorf, K. Sokolowski-Tinten, S. Schlücker, J. of Phys. Chem. C 123, 13181 (2019).

P. Zalden, F. Quirin, M. Schumacher, J. Siegel, S. Wei, A. Koc, M. Nicoul, M. Trigo, P. Andreasson, H. Enquist, M. Shu, T. Pardini, M. Chollet, D. Zhu, H. Lemke, I. Ronneberger, J. Larsson, A. M. Lindenberg, H. E. Fischer, S. Hau-Riege, D. A. Reis, R. Mazzarello, M. Wuttig, K. Sokolowski-Tinten, Science 364, 1062 (2019).

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Research Topic

Quantum Transport of Charge and Heat

- Mesoscopic thermoelectrics
- Phase-coherent heat transport
- Unconventional superconductivity

Selected Publications

S. R. Valentin, J. Schwinger, P. Eickelmann, P. A. Labud, A. D. Wieck, B. Sothmann, A. Ludwig, Phys. Rev. B 97, 045416 (2018).

S.-Y. Hwang, P. Burset, B. Sothmann, Phys. Rev. B. 98, 161408(R) (2018).

G. Jaliel, R. K. Puddy, R. Sanchez, A. N. Jordan, B. Sothmann, I. Farrer, J. P. Griffiths, D. A. Ritchie, C. G. Smith, Phys. Rev. Lett. 123, 117701 (2019).

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Research Topic

Materials and Devices for Nanoelectronics and -photonics

- Nanoscale semiconductor materials - growth and characteristics
- Electronic/optoelectronic device design, fabrication, characterisation and modelling
- Nanointegration technologies for electronics and photonics

Selected Publications

L. Liborius, J. Bieniek, A. Nägelein, F.-J. Tegude, W. Prost, T. Hannappel, A. Poloczek, N. Weimann, Phys. Status Solidi B (2019).

C. Speich, F. Dissinger, L. Liborius, U. Hagemann, S. R. Waldvogel, F.-J. Tegude, W. Prost, Phys. Status Solidi B (2019).

L. Liborius, F. Heyer, K. Arzi, C. Speich, W. Prost, F.-J. Tegude, N. Weimann, A. Poloczek, Phys. Status Solidi A 216 (2019).

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Research Topic

Functional Polymer Materials

- Membranes and membrane-based technologies
- Molecularly imprinted polymers (MIPs), stimuli-responsive polymers
- Surface functionalization of materials

Selected Publications

C. Alexowsky, M. Bojarska, M. Ulbricht, Journal of Membrane Science 577, 69 (2019).

A. Wittmar, Q. Fu, M. Ulbricht, Cellulose, 26, 4563 (2019).

M. Ulbricht, RSC Smart Materials Series 35, 297 (2019).

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Research Topic

Biosupramolecular Chemistry

- Materials for medical and biological imaging
- Self-assembly of amohiphiles
- Novel photosensitizers
- Transfection agents

Selected Publications

M. Hayduk, S. Riebe, K. Rudolph, S. Schwarze, F. van der Vight, C. G. Daniliuc, G. Jansen, J. Voskuhl, Isr. J. Chem. 58, 927 (2018).

J. Stelzer, C. Vallet, A. Sowa, D. Gonzales Abradelo, S. Riebe, C. Daniliuc, C. Strassert, S. Knauer, J. Voskuhl, ChemistrySelect 3, 985 (2018).

S. Riebe, M. Saccone, J. Stelzer, A. Sowa, C. Wölper, K. Soloviova, C. A. Strassert, M. Giese, J. Voskuhl, Chem. Asian. J. 14, 814 (2019).

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Research Topic

Devices for Ultrahigh Frequency (UHF) Electronics and Photonics

- Epitaxy of semiconductor materials for UHF applications
- Design, fabrication, characterization, and modelling of UHF devices and their integration in circuits and modules
- Heterogeneous materials integration for UHF devicess

Selected Publications

N. G. Weimann, T. K. Johansen, D. Stoppel, M. Matalla, M. Brahem, K. Nosaeva, S. Boppel, N. Volkmer, I. Ostermay, V. Krozer, O. Ostinelli, C. R. Bolognesi, IEEE Transactions on Electron Devices 65, 3704-3710 (2018).

L. Liborius, F. Heyer, K. Arzi, C. Speich, W. Prost, F.-J. Tegude, N. Weimann, A. Poloczek, physica status solidi (a) 216, 1800562 (2018).

C. Blumberg, S. Grosse, N. Weimann, F.-J. Tegude, W. Prost, physica status solidi 255, 1700485 (2018).

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Research Topic

Element specific Magnetic Properties of Nanostructures

- Magnetic bio-molecules on surfaces
- Ultrathin films and their interfaces for spintronic devices
- Magnetic anisotropy, orbital and spin moments of magnetic nanoparticles
- Magnetic coupling phenomena in nanostructures

Selected Publications

F. Huttmann, [...], O. Eriksson, W. Kuch, T. Michely, H. Wende, J. Phys. Chem. Lett. 10, 911 (2019).

K. Chakrapani, [...], R. Schlögl, H. Wende, R. Pentcheva, S. Schulz, M. Behrens, ACS Catalysis 8, 1259 (2018).

F. Scheibel, T. Gottschall, A. Taubel, M. Fries, K. P. Skokov, A. Terwey, W. Keune, K. Ollefs, H. Wende, M. Farle, M. Acet, O. Gutfleisch, M. E. Gruner, Energy Technol. 6, 1392 (2018).

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Research Topic

Nanoparticles and Nanomaterials

- Synthesis of nanoparticles in the gas phase
- Impedance spectroscopy of nanomaterials/solid state sensor materials
- Electrical properties of mesoscopic systems

Selected Publications

G.-L. Xu, L. Xiao, T. Sheng, J. Liu, Y.-X. Hu, T. Ma, R. Amine, Y. Xie, X. Zhang, Y. Liu, Y. Ren, C.-J. Sun, S.M. Heald, J. Kovacevic, Y. H. Sehlleier, C. Schulz, W.L. Mattis, S.-G. Sun, H. Wiggers, Z. Chen, K. Amine, Nano Lett. 18, 336 (2018).

B. Alkan, S. Cychy, S. Varhade, M. Muhler, C. Schulz, W. Schuhmann, H. Wiggers, C. Andronescu, ChemElectroChem 6, 4266 (2019).

C. Schulz, T. Dreier, M. Fikri, H. Wiggers, Proc. Combust. Inst. 37, 83 (2019).

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Research Topic

Electrochemical Energy Storage and Conversion

- Development of new materials, components, and cell design
- Lithium-ion batteries
- Lithium-metal systems (solid, sulfur, air, etc.)
- Dual-ion batteries
- Super capacitors (including lithium-ion capacitors)
- Alternative lithium-free systems

Selected Publications

R. Schmuch, R. Wagner, G. Hoerpel, T. Placke, M. Winter, Nat. Energy 4, 267–278 (2018).

J. Betz, G. Bieker, P. Meister, T. Placke, M. Winter, R. Schmuch, Adv. Energy Mater. 9, 6 (2018).

M. Winter, B. Barnett, K. Xu, Chem. Rev. 118, 11433-11456 (2018).

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Research Topic

Nanoparticle Process Technology

- Functional nanomaterials
- Nanoparticle synthesis and processing
- In-situ Process analysis
- Structural characterization

Selected Publications

S. M. Ognjanovic, M. Zähres, C. Mayer, M. Winterer, J. Phys. Chem. C 122, 23749 (2018).

J. S. Gebauer, V. Mackert, S. Ognjanovic, M. Winterer, J. Colloid Interface Sci. 526, 400 (2018).

M. Winterer, Chem. Eng. Sci. 186, 135-141 (2018).

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Research Topic

Modelling and Simulation: Reaction Kinetics, Aerosol Dynamics, and Fluid Mechanics

- Simulation of chemically reacting and particle building fluids in flames and reactors
- Development, optimization, and reduction of reaction mechanisms
- Numerical solution methods for conservation equations

Selected Publications

H. Janbazi, Y. Karakaya, T. Kasper, C. Schulz, I. Wlokas, S. Peukert, Chem. Eng. Sci. 209, 115209 (2019).

F. Schneider, S. Suleiman, J. Menser, E. Borukhovich, I. Wlokas, A. Kempf, H. Wiggers, C. Schulz, Rev. Sci. Instrum. 90, 085108 (2019).

J. Sellmann, I. Rahinov, S. Kluge, H. Jünger, A. Fomin, S. Cheskis, C. Schulz, H. Wiggers, A. Kempf, I. Wlokas, P. Combust. Inst. 37, 1241 (2019).

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Research Topic

Computational and Statistical Physics

- Non-contact friction (dynamic force microscopy)
- Magnetic friction, nonlinear mesoscopic friction
- Sintering of nano-particles
- Impedance of particle networks
- Conductance of nano-powders
- Epitaxial growth

Selected Publications

M. Jongmanns, R. Raj, D. E. Wolf, New J. Phys. 20, 093018 (2018).

T. Stegmann, O. Ujsaghy, D. E. Wolf, New J. Phys. 20, 043039 (2018).

I. A. Okanimba Tedah, F. Maculewicz, D. E. Wolf, R. Schmechel, J. Phys. D: Appl. Phys. 52, 275501 (2019).

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Research Topic

Nanoparticles and Phase Boundaries

- Interactions of nanoparticles with biomolecules
- Uptake of nanoparticles on liquid surfaces
- Optical tweezing
- SERS spectroscopy

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Research Topic
Surface Nanolayers
- Wear and friction of metallic materials
- Nanotopography and structuring
- Micro- and nanostructural analyses

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Research Topic
Ferroic Multifunctional Materials
- Ab initio and ab initio based modeling
- Ferroelectrics, ferromagnets, and multiferroics
- Ferroic cooling

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Research Topic
(Nano-)Photonic Components and Systems
- Photovoltaics and solar cells
- Fibre, wireless and optical communications
- Microwaves and THz technology
- Sensors and security
- LEDs for illumination

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Research Topic
Integrated Micro- and Nanosystems
- Physical sensor/actuator systems
- Atom and ion chips – manipulation of atoms and ions

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Research Topic

Laser generated Nanoparticles for Catalysis

- Laser based synthesis of catalytic active nanomaterials in solution
- Nanoparticle processing (size and surface modification, particle separation)
- Upscaling and application in heterogeneous catalysis

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Research Topic

Nanophotonics and Nanomaterials

- Spectroscopy on nanostructured materials
- Advanced semiconductor nanopatterning techniques
- Nanophotonic devices for the visible spectral range

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Research Topic

Oxide Spintronics

- Nanoscale Oxide Materials
- Magnetic and electronic interface phenomena
- Synchrotron-based spectroscopy

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Research Topic

Magnetic Semiconductors

- Dilute magnetic semiconductors
- Heterostructures for magnetotransport and magnetic logic
- Nanoclusters and their interactions in semiconducting hosts

Former CENIDE Members

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Research Topic

Nanomaterials for Electronic Devices

- Thermoelectrics
- Nanoparticle sintering

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Research Topic

Nanobased heterogeneous catalysis

- Nano-based photocatalysis for energy storage
- Structure-function relationships of heterogeneous photocatalysts
- Surface doping of catalysts
- Infrared spectroscopy and adsorption of probe molecules

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Research Topic

(Nano-)Photonic Components and Systems

- Photovoltaics and solar cells
- Fibre, wireless and optical communications
- Microwaves and THz technology
- Sensors and security
- LEDs for illumination

Publishing details

Published by
CENIDE – Center for Nanointegration Duisburg-Essen

Project management
Steffi Nickol, M.Sc.,
and Dipl.-Biol. Birte Vierjahn

Editors
Prof. Malte Behrens, Steffi Nickol, M.Sc.,
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Dipl.-Biol. Birte Vierjahn, Prof. Heiko Wende

Layout
Melanie Daamen, Steffi Nickol, M.Sc.
Paran Pour, Studio Ra

Frequency
Biennially

Printed by
Universitätsdruckzentrum, 3rd Edition

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A Journal of CENIDE –
Center for Nanointegration Duisburg-Essen
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